# Hydrogen as an Energy Product from Agriculturally Produced Sugars and Starches in South Africa

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# Declaration

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# Synopsis

Bio-fuels have a significant role to play in the South African energy economy. They have a potential to impact positively on the quality of life of a large number of people while providing environmental gains geared at addressing environmental challenges such as global warming. Technologies to produce bio-fuels are well established and processes mature, however energy yields are low to modest in relation to land used. More efficient technologies, the so called 'second generation bio-fuels technologies' are being developed in response to this challenge. On a parallel track, research to enable the 'hydrogen economy' is also being stimulated. This dissertation investigates the potential transfer of a 'second generation bio-fuel technology' developed elsewhere into the South African industry. The technology of interest is called Aqueous Phase Reforming (APR) and it is claimed to provide an efficient route for hydrogen production from intermediate process sugar streams. The main questions that guide the thesis are as follows:

- Which industries would be best suited to produce and use hydrogen from maize or sugar? Both power and liquid fuels sectors are included in the analysis.

- Does the higher energy efficiency of APR translate into a life cycle environmental advantage? This is approached using Life Cycle assessment (LCA) of bioenergy products made from maize starch.

- How do the environmental impacts of the different industrial applications compare?

The questions are addressed with aid of a literature review, followed by a Life Cycle Assessment of generated industrial options. The literature review serves to inform about the status quo of bio-energy technology and explores similar studies on LCA of bio-energy systems. It also identifies, in addition to a new maize-based fuel ethanol sector, the existing cane sugar and emerging biodiesel processing as industries into which the APR could be transferred.

A range of industrial options are developed for the energy products ethanol and hydrogen produced from hydrolyzed maize starch. These options are divided into two broad industrial applications of power generation and transportation, whose merit is then investigated. An environmental life cycle assessment investigates the sustainability benefits of 8 developed industrial options defined as follows: ethanol for peak power generation with or without heat integration (EE and EE-HI), hydrogen for peak power generation with and without heat integration (HE and HE-HI), ethanol for use in a Flexi-Fuel Vehicle (E-FFV) and Fuel Cell Vehicle (E-FCV) and hydrogen use in an ICE vehicle and a Fuel Cell Vehicle ($H_2$-ICEV and $H_2$-FCV). The LCA results are evaluated on the following impact indicators: Global Warming, Human Toxicity, Fresh Water Eco-toxicity, Acidification and Eutrophication. For the comparison of electrical and transportation energy products an LCA technique called system boundary expansion (as recommended by the ISO standard on LCA) is used.

The results demonstrate that the APR hydrogen options would out-perform the classic fermentation and distillation ethanol options for electricity and transportation options by outscoring them in all impact categories studied. Process heat integration for the electricity options would improve the environmental performances of these options drastically on the one hand, while technology improvement in the form of fuel cell vehicles also would improve the performance of the transport options. The comparison of peak power generation options and transportation options shows the superiority of the electricity options in all but one of the impact categories studied. The results resonate with the general wisdom emerging from LCA literature that limited renewable energy should always be targeted at replacing the "dirtiest fuel in the system".

The transportation options generally show a poorer environmental performance. It was therefore thought worthwhile to consider another option that might present better environmental gains. It is investigated conceptually how the APR process could be incorporated into the coal-to-liquid-fuels process to primarily reduce the carbon dioxide emissions and additionally produce more gasoline, translating into additional vehicle transportation service. When system boundaries are expanded for comparison with the other four transportation options, this option performs very closely to the E-FCV, outscoring only the E-FFV, but performing poorer than the hydrogen options.

Based on the findings of the study, short to medium options and long term options are recommended. Peak power generated from ethanol is envisaged for short term while that from hydrogen was foreseen for medium term because of its environmental benefits and the relative ease of implementation compared to the efficient transport options. Heat integration into peak power generation options presents attractive environmental performance and needs to be analysed and investigated further. Although seen not to have much of an edge over the other transportation options the APR incorporation into coal to liquid process could better the environmental performance of this industry. This presents a medium term option because of the relative ease of implementation in comparison with the most efficient hydrogen transportation options. Long term options include $H_2$-FCV if coal based electricity is replaced by other renewables because fuel cell vehicles present better environmental gains than the internal combustion engine vehicle.

# Dedication

This thesis is dedicated to my parents 'Marethabile and the late Mokhatla Melamu for their immeasurable sacrifices, support and motivation for the sake of my academic endeavours. Thank you.

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# Glossary

The major terms used in this thesis are listed below:

| | |
|---|---|
| CTL-$H_2$ | A coal to liquid process transportation option which produces additional kilometres |
| EE | Peak power generation option using ethanol |
| EE-HI | Same as EE but has heat integration into the distillery |
| E-FCV | Transportation option using ethanol in a fuel cell vehicle |
| E-FFV | Transportation option using ethanol in a flexi-fuel vehicle |
| $H_2$-FCV | Transportation option using hydrogen in a fuel cell vehicle |
| $H_2$-ICEV | Transportation option using hydrogen as fuel in an internal combustion engine vehicle |
| HE | Peak power generation option using hydrogen |
| HE-HI | Same as HE with heat integration into the APR process |
| LCA | Life Cycle Assessment |
| LCI | Life Cycle Inventories |
| LCIA | Life Cycle Impact Assessment |

# 1 Introduction

## *1.1 Background*

Dependence on fossil fuels as the main energy sources has its attendant problems, including the unsustainable depletion of fossil fuel reserves, the increase of carbon dioxide in the atmosphere driving climate change and emission of pollutants. In response to these problems, continuous effort is being directed to the exploration of clean, renewable alternatives for sustainable development. Biomass is considered a promising sustainable energy source because of the possibility of continual replenishment, the relative ease of harnessing it, and the local economic benefit created. However, one of the major drawbacks of using biomass as an energy source is the risk of expansion of mono-culture croplands causing loss of biodiversity, caused in part by the low biomass-to–energy conversion efficiency. New biomass to energy technologies that have higher yields and efficiencies are being developed for better exploitation of biomass resources.

Fuel cells have emerged as promising devices for meeting the needs of higher conversion efficiency and lower (or zero) emissions. These cells use hydrogen and are clean, quiet and efficient devices for electric power generation (Davda *et al.*, 2005). However the development of concepts for low-cost large scale environmentally sustainable systems for hydrogen production remains a challenge. One set of possible options revolves around the conversion of relatively abundant and cheap biomass. Processes like enzymatic decomposition of sugars, steam reforming of oils or gasification are considered, but entail low hydrogen production rates and/or complex processing requirements (Garcia *et al.*, 2001). The production of hydrogen for fuel cells and other industrial applications from renewable biomass thus remains a major challenge as the world moves towards a 'hydrogen society' (Davda *et al.*, 2005).

In this light, a recently developed technology is of interest. It converts carbohydrates such as sugars and polyols with water, in aqueous phase over an appropriate heterogeneous catalyst at temperatures close to 500 K to primarily produce hydrogen and carbon dioxide (Cortright *et al.*, 2002). This process is called Aqueous Phase Reforming (APR) and it provides an efficient route for hydrogen generation

from aqueous phase carbohydrates found in waste water from biomass processing (e.g. from brewery waste water and sugar processing) and from streams extracted from agricultural products such as maize and sugar beet (Cortright *et al.*, 2002).

The South African government is beginning to show some commitment to the establishment of a biofuels industry as an initiative to realise its target of 10 000 GWh of renewable energy penetration into the energy sector by 2013 (White Paper on Renewable Energy, 2003). To help foster the growth of this industry the Department of Minerals and Energy has finalised the Biofuels Industrial Strategy outlining the government's approach to addressing policy, regulations and incentives. The biofuel strategy aims to achieve a biofuel average market penetration of 2% (by volume) of liquid transport fuels in the country by 2013 (Industrial Biofuel Strategy, 2007).

The Department of Science and Technology's (DS&T) proposal to promote hydrogen and fuels cell as priority technologies for reducing the country's dependence on fossil fuel has also been recently approved by the cabinet. The department views such a 'hydrogen economy' as an opportunity for harnessing more sustainably the country's natural resources while yielding multiple social and economic benefits (Department of Science and Technology Annual Report, 2005/6). Production of hydrogen especially from renewable resources is one of the areas that are critical to the development of this economy.

Currently, South Africa does not have enough capacity for electricity generation to meet the increasing demands; this has been evident from the number of blackouts that have been experienced throughout the country in the past two years. The situation is likely to worsen in the near future because of the economic growth and the government's mandate to make electricity available to all. It is predicted that it would take about 6 years to complete building the next base load coal station to match the increasing demand and that it might even take 10 years or more to acquire the safe reserve margin (Kenny, 2007). Power generation from renewable sources presents an opportunity that could increase capacity and better the environmental performance of the country's intensive coal based power generation.

The biofuel strategy targets an average market penetration of 2% of liquid transport fuels, if blending is made mandatory for oil companies they would be obliged to absorb most of the biofuel volumes. The oil companies could opt to utilise biofuels for other applications besides blending into fossil fuels. Electricity generation for peak power needs is one option that can be exploited by the oil companies. It is possible to generate electricity by combusting bio-ethanol or bio-diesel instead of blending it into motor fuel.

Whilst biofuels are promoted by the government primarily for their job creation potential, the environmental benefits should not be forgotten. In view of the possibility of using bio-ethanol for power generation, it is therefore important to recall that South Africa's coal-based electricity is highly polluting, as shown by a comparative study of air emissions of thermal power plants of 15 European countries with those found in South Africa (von Blottnitz, 2006). These countries do not only include those that have developed technologies such as Germany and the UK, it also has countries that have less developed technologies such as Poland. In this study four specific emissions were considered; $NO_x$, $SO_x$, $PM_{10}$ and $CO_2$. From the results it was shown that $NO_x$ and $SO_X$ emissions appear to fall into three broad categories; those with stringent pollution control, those with some pollution control and those with very little pollution control. The emission results which were presented in g/kWh of electricity generated showed South Africa to fall under the latter category with the highest relative and absolute emissions of $NO_x$ and $SO_x$ compared to all the 15 European nations, and with the 3$^{rd}$ largest power-related $CO_2$ emissions of the 16 compared countries.



Research on upcoming technologies will be needed to enable South Africa to move beyond its 2013 10 000 GWh target of renewable energy. This thesis aims to explore one such technology, Aqueous Phase Reforming (APR).

## *1.2 Problem statement*

Increased environmental regulations on fossil fuels emissions and global warming mitigation strategies have led to much R&D on alternative forms of sustainable energy, mostly renewable energy. Biomass is considered a promising sustainable energy source which can be harnessed with relative ease. However, one of the

drawbacks associated with its utilisation is the low efficiencies associated with its conversions to energy carriers.

In South Africa, maize and sugar cane are the two highest yield agricultural products, and both can be converted to bio-ethanol. There is a potential industrial interest in the production of ethanol from maize, a conversion route characterised by modest energetic yields at ~400 litres of ethanol per ton of maize, or 0.55 MJ in ethanol per MJ in maize on an energetic (LHV) basis[1]. However the same intermediate sugar streams in the maize-ethanol process route could potentially be converted into hydrogen by aqueous phase reforming (APR), at a theoretical yield of ~100 kg $H_2$ per ton of maize (Virent Inc, 2006), or 0.71 MJ in hydrogen per MJ of maize.

Considering the existence of this novel technology (APR) in the light of both the government's short-term renewable energy target as well as its longer-term S&T ambitions w.r.t. hydrogen; an opportunity has been realised to explore the environmental merit of the APR process in South Africa. The problem or opportunity to be investigated by this thesis can be summarised as follows:

'Based on its claimed higher energetic yield than the fermentation-distillation route, and given that Aqueous Phase Reforming (APR) could form a stepping stone into the hydrogen economy, potential applications in the existing or future energy and fuels markets in South Africa need to be explored.'



## *1.3 Objectives*

Based on the problem statement the work presented in this thesis aims to achieve the following objectives:

i) To analyse the potential transfer of the APR technology into suitable industrial sectors in South Africa. One such industry is the nascent biofuels sector. It is claimed that hydrogen could be produced via aqueous phase reforming of intermediate streams in the maize to ethanol process at higher energetic yields than ethanol. Another industry is the

[1] Calculations in Appendix A1

sugar milling industry where the development of alternative revenue generating opportunities is of high importance. Feedstocks include excess export sugar, impure sugar process streams and molasses. The nascent biodiesel industry also presents a good opportunity for APR where glycerol by-product could be used as a suitable feedstock.

ii) To explore the environmental implications of employing this technology to produce hydrogen as an energy product from agriculturally produced sugars and starches in South Africa. It is advisable to investigate the environmental implications of such a new industrial configuration prior to suggesting any further R&D aimed at establishing the APR technology.

## *1.4 Key questions*

The key questions that are addressed by the dissertation include:

a) Which industries would be best suited to produce and use hydrogen from maize, sugar or glycerol? Both power and liquid fuels sectors will be included in our analysis.

b) Does the higher energy efficiency of APR translate into a life cycle environmental advantage? This will be approached using Life Cycle assessment (LCA).

c) How do environmental impacts of the different industrial applications compare? This will be addressed by employing system boundary expansion in their comparison.

Previous work has focused mostly on the underlying science, and the technical implementations of the Aqueous Phase Reforming technology (Cortright *et al.*, 2002, Shabaker *et al.*, 2003, Davda *et al.*, 2005) . This dissertation takes more of an industrial strategy direction, working with sustainability assessment tools, in the context of the resource-industry intensive nature of the South African economy.

## *1.5 Hypothesis*

The hypothesis developed at the beginning of the thesis is stated as follows:

> Using energy products derived from maize for peak power generation as opposed to vehicle fuel is environmentally attractive in South Africa because the coal based electricity has a high environmental impact.

## *1.6 Methodology*

The first task is to present a review of the literature pertaining to previous and novel bioenergy technologies, especially on APR. This will help establish knowledge of the APR technology to the reader, by presenting what is potentially possible. It also seeks to help identify suitable industrial sectors for the technology's transfer into South Africa.

The second task is to review literature on recent advances in environmental assessment of technologies, in particular in the field of Life Cycle Assessment as applied to bioenergy technologies. This will help to refine the initial hypothesis.

Thirdly, a range of scenarios will be developed for the production of ethanol or hydrogen from maize and their subsequent use in transport or electricity generation. These scenarios will then be evaluated in a comparative Life Cycle Analysis. These scenarios are divided into two broad industrial applications of power generation and transportation whose merit will be investigated. This will deliver insights expected to be in support of the hypothesis.

## *1.7 Scope*

This dissertation presents an analysis of Aqueous Phase Reforming, as well as of industrial sectors in South Africa that might be interested to employ it. It then explores major aspects towards a better understanding of factors and implications of employing this technology to produce hydrogen as an energy product from agriculturally produced sugars and starches in South Africa. The analyses presented here are not based on laboratory experimental work; most of the analysis involves

flow-sheeting with Microsoft Excel, and Life Cycle Assessment with an LCA software package.

## *1.8 Thesis outline*

Based on a realised opportunity and the developed key questions, a review of the literature will be carried out in Chapter 2. Chapter 3 will explore the methodology and approach followed for the research. A Life Cycle Assessment for the transport and power generation scenarios is presented in Chapter 4. Chapter 5 explores the use of hydrogen generated via Aqueous Phase Reforming in a petro-chemical industrial complex emitting large amounts of carbon dioxide. Conclusions are drawn and then recommendations are made in Chapter 6.

# 2 Literature Review

This chapter aims to elaborate the background to the work presented in this dissertation, and review published work that it is both relevant to and in line with the aims and objectives of the study.

The value of the work presented in this dissertation is anchored in the role that the South African agricultural sector could potentially play in support of the development of a national biofuels industry; an overview of this agricultural sector is thus sketched out first. This is followed by a review of bioenergy technologies, discussing some of the conventional biomass to bioenergy conversion technologies, followed by a discussion on the sustainability of the maize-to-ethanol conversion route. Some examples of 2nd generation bioenergy conversion technologies are then introduced, followed by a more detailed review of the technology under investigation, Aqueous Phase Reforming (APR). Prior work involving life cycle assessment of 2$^{nd}$ generation technologies is then reviewed in the context of a discussion on LCA and its different variations, and finally conclusions are drawn.

## *2.1 The South African biofuel policy context*

The utilisation of biomass as an energy feedstock is increasing in many countries and is seen as a step towards sustainable development. In South Africa in particular, there is much political and economic interest to move towards agriculturally produced biomass for energy products to address the effect which the increasing crude oil price will have on the pump price of fuels and on the national balance of payments, with future pressures to mitigate fossil carbon dioxide emissions as well as rural economic development being further considerations. There is a concern in the government that the sharp and sustained rise in fuel price would have a negative impact on the economy.

The government is thus under pressure to support various renewable energy endeavours, such as bio-fuels. For instance, it has been found that one of the ways to achieve this goal is to encourage farmers to plant energy crops on a large scale to be used as feedstock for bio-fuels products. In order to achieve this goal, available agricultural land needs to be exploited efficiently. South Africa has limited arable land, with only 14% of the total land being suitable for production of crops;

however, there is still about 3 million hectare of currently underutilised high potential land mainly lying in the former homelands (Biofuel Industrial Strategy, 2007). It is claimed that utilising 1 million hectare of such land could produce about 5% of national diesel usage (Biofuel Industrial Strategy, 2007). The climate patterns and agricultural zones in South Africa are important aspects to understanding the yields and production of the biofuel crops as well as potential locations for biofuel industries.

South Africa has an average annual rainfall of 500 mm, with more than 80 percent of its land surface classified as semi-arid to arid according to the United Nations Council on Combating Desertification (UNCCD). Only 18 percent is classified as dry sub-humid and sub-humid, hence suitable for rain-fed crop production of which biofuel crops forms part of (FAO, 2005). Cereal crops such as maize and wheat are grown in the summer rainfall regions of the Free State, Mpumalanga and North West while sugar cane is grown in Mpumalanga and kwaZulu-Natal. Maize is a dominant crop with an average production of 7 million tonnes per annum for 2005/06 (www.grainsaa.co.za) followed by sugar cane with the production of 2 million tonnes per annum of sugar for 2005/06, both of which can be utilised for the production of bioethanol. In recent years there has been surplus maize and sugar cane that could produce ethanol at more than 5% national petrol demand (Draft Biofuel Industrial Strategy, 2006).

The government is coming up with policies that are geared at addressing the issues discussed above, for an example, the policy on renewable energy that envisages a range of measures essential to bring about the integration of renewable energies into the mainstream energy economy. To achieve this, the government has set a target of 10 000 GWh renewable energy contribution to final consumption by 2013 to be produced mainly from biomass, solar, wind and small scale hydro power (White Paper on Renewable Energy, 2003). The latest initiative by the government towards the 2013 renewable energy target is the development of its industrial strategy on the commercialisation of biofuels, which was approved by Cabinet in December 2007. The release of the draft strategy for comment in December 2006 stimulated a lively discussion amongst stakeholders. Somewhat separate from these two implementation oriented strategies of government is its science and technology strategy for the hydrogen economy.

The South African cabinet approved the proposal of the Department of Science and Technology to promote hydrogen and fuel cell economy as priority technologies to reduce the country's dependence on fossil fuel in June 2005. The strategy is aimed at developing the necessary human resource capacity required to building on knowledge. The Department of Science and Technology views the hydrogen economy and its related fuel cell technologies as a leading 'Frontier Science and Technology' area that could potentially change the country's natural resource dependence while yielding multiple social and economic benefits (Department of Science and Technology, 2005).

To achieve the desired benefits without significant negative social and environmental consequences, the government's bio-fuels initiative needs to be aware of the limitations of the energy systems that can convert biomass efficiently into energy carriers and services. One of the problems with the first generation modern biomass to biofuel conversion systems revolve around the limited efficiencies of the conversion processes or the limited feedstock range they can process (McKendry, 2002). Another problem centres on the extensive use of fossil energy in the bioenergy supply chain to an extent that the climate-change mitigation aspiration maybe largely negated (von Blottnitz and Curran, 2007).



## *2.2 Bioenergy conversion systems*

This section reviews some of the relatively low efficiency conventional biomass to energy technologies. It is followed by a more detailed discussion of these limitations in the light of starch-fed ethanol production systems. This is then followed by an introduction to some examples of the emerging biomass to energy conversion technologies that claim higher efficiencies.

### 2.2.1 Conventional biomass to bioenergy conversion routes

The field of biomass to energy technology has been attracting a 2$^{nd}$ wave of R&D interest in the wake of climate change concerns (the 1$^{st}$ wave was in response to the oil price shocks of the 1970s), and some technologies have been used on a large industrial scale for a number of years. Most of these technologies have low

efficiencies; however they are being constantly improved to gain higher efficiencies. Some of these technologies are outlined below.

### 2.2.1.1 Thermo-chemical conversions

Three major processes are used for thermo-chemical conversion of biomass.

***Combustion***

Combustion conventionally implies the direct burning of biomass in air to convert the biomass chemical energy into heat, which may be converted to mechanical power and electricity. Equipment such as stoves, furnaces and fluidised bed boilers convert the feedstock to heat, and steam turbines or gas turbines may be employed to produce mechanical power which can then be used to drive electrical generators. The combustion of air produces hot gases at temperatures of about 800-1000 $^{0}$C. This type of conversion is more suited for biomass that has a moisture content of less than 50%. The scale of combustion ranges from a very small scale (e.g. domestic heating) up to large industrial scale in the range of 100-3500 MW. The net conversion efficiency for biomass to electricity conversion plants is between 20% and 40%, (McKendry, 2002). New developments in combustion technology (such as oxyfuel combustion or chemical looping combustion) are driven by an interest to produce concentrated or pure carbon dioxide streams for sequestration.

***Gasification***

Gasification is the conversion of biomass into a combustible mixture of gases by partial oxidation at high temperatures typically in the range 1000-1200K. The product gas can be used as a feedstock (syngas) to produce chemicals (e.g. methanol, hydrocarbons) or fuels (gasoline or diesel). Gasification can be integrated with combustion to convert the produced gases in turbines to electricity with high overall conversion efficiencies of about 40-50%, (McKendry, 2002). The production of syngas from biomass also allows for the subsequent recovery of hydrogen, which may have future as an energy product. Large scale biomass gasification has so far been relatively unsuccessful due to both technical difficulties and cost barriers. A good example is that of a patented biomass gasification technology called Carbon-V by CHOREN industries which produces a type of diesel called Sun-Diesel. This biomass to liquid (BTL) technology is still to be applied on a large scale because

of a range of challenges such as higher investment costs, lack of reference plants, a higher risk of any form of investment, earlier learning curves associated with higher production costs (Rudloff, CHOREN industries, 2007).

***Chemical modification of oils and fats into biodiesel***

The production of biodiesel from oil crops and other feedstocks has been growing in importance in the recent years. Biodiesel is produced through a process called transesterification, where vegetables oils or animal fats (triglycerides) react with an alcohol (e.g. methanol, ethanol) in the presence of a catalyst, usually a strong base, such as sodium or potassium hydroxide, however acid and enzyme catalysts can also be used. The products are known as fatty acid alkyl esters, it is these esters that have come to be known as biodiesel. One major by-product of the transesterification process is glycerine. The biodiesel reaction is presented by the equation below:

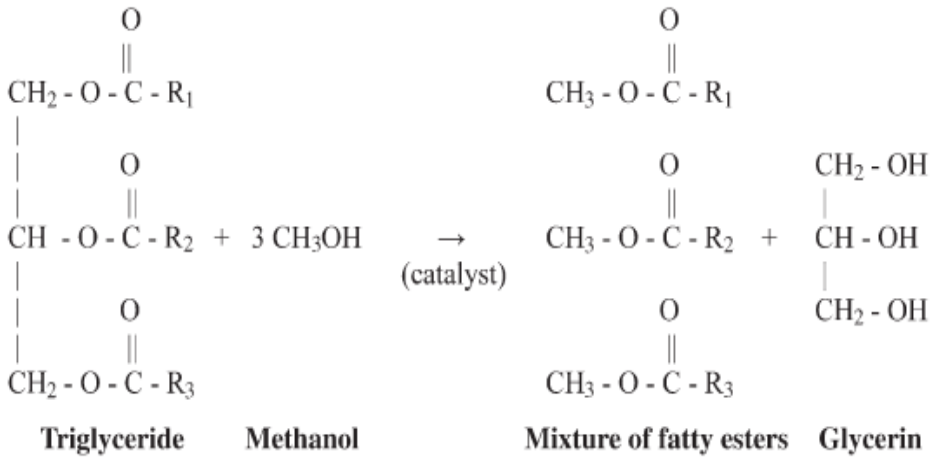


**Figure 2.1: The biodiesel reaction equation (Kadpan, 2006)**

Biodiesel is already being produced on a large scale in some countries, for instance, Germany. The South African draft industrial biofuels strategy has proposed a 2% market penetration target for the year 2013 (Biofuel Industrial Strategy, 2007).

### 2.2.1.2 Biological conversions

Two main bio-chemical processes are practiced extensively, anaerobic digestion of organic waste into biogas and fermentation of sugars into ethanol (sometimes after hydrolysis of starches).

***Anaerobic Digestion***

AD is the breakdown of the organic matter by bacteria in the absence of oxygen directly into biogas, which is a mixture of mainly methane and carbon dioxide and a trace of other gases such as hydrogen sulphide (Themelis, 2006). The other by-product is slurry that it is rich in nutrients and can be used as fertilizer depending on the organic material digested. AD is a commercially proven technology that treats biomass with a high moisture content of over 80% (McKendy, 2002). Biogas can be used directly in boilers or gas turbines and can be upgraded to a higher quality i.e. natural gas quality by the removal of carbon dioxide. It can be used for the generation of industrial heat, electricity, or combined heat and power, or even to drive cars.

***Fermentation***

Fermentation is a process used commercially on a large scale to produce ethanol from sugar crops (e.g. sugar cane, sugar beet, molasses) or starch crops (e.g. maize, wheat). In the processing of starch-containing seeds, the feedstock is ground and the starch converted to sugars by enzyme-assisted hydrolysis at elevated temperatures. The yeast then converts the sugars to ethanol in a fermentation vessel. The normal practice is to use the solid residue from fermentation as cattle feed. The possibility of converting lignocellulosic biomass is becoming more attractive (Kadpan, 2006), however it is more complex due to the presence of longer polysaccharide molecules and requires enzymatic or acid hydrolysis before the sugars can be fermented to ethanol.



The section below looks at some of the limitations of the first generation bioenergy technologies in the light of starch-fed ethanol production.

## 2.2.2 Sustainability of the maize to ethanol route

Many studies have been published on the aspects of environmental sustainability of the maize to ethanol conversion route, most focussing on the 'energy balance' issue, some on greenhouse gas emission reductions, and a few using Life Cycle Assessment. In their assessment of 47 publications on bio-ethanol systems, von

Blottnitz and Curran (2007) identified some important limitations of the current industrial practice, and in sustainability analysis that are summarised below.

They divided their results on the environmental sustainability of producing ethanol from maize into three categories; 1) reducing the dependence on fossil fuel through energy balance assessments, 2) reducing emissions on green house gases and 3) reducing health and environmental impacts through the life cycle.

Energy balance assessment was found to be reported in one of two categories, the net replaced fossil fuel and energy yield ratio. The net replaced fossil fuel was measured relative to land area used. For maize in North America, a fossil energy replacement of 38 GJ/ hectare-annum appears to be an accepted result. McKendry (2002) and EU (1999) also reported a close figure of 39 GJ/hectare-annum, a very poor performance compared to sugar crops, whose replacement was much higher, e.g. Brazilian sugar crops have a replacement of about 250 GJ/hectare-annum (von Blottnitz and Curran, 2007).

In terms of energy yield, a ratio that relates energy output of fossil fuel energy to the energy input into its production, it was found that the energy yield ratio for maize to ethanol ratio is just marginal at about 1.3, a low figure compared to the 7.9 of Brazilian sugarcane to ethanol (von Blottnitz and Curran, 2007). Pimentel and Patzek (2005) disagree with most other published work on North-American maize-ethanol, reporting that maize requires 29% more fossil energy than the fuel produced. Farrell et al. (2006) have pointed out methodological inconsistencies in this work, and arrive at a result consistent with that of von Blottnitz and Curran (2007). In assessing the energy input, one considers energy used in producing the crop (e.g. production of pesticides and fertilizers, grinding and transporting of the crop) and energy used in fermenting and distilling ethanol from the water mix.

On the issue of greenhouse gases, it was observed that the starch-based ethanol systems produce more greenhouse gases, due to their intensive use of fossil fuel in the bio-fuel production compared to the sugar to ethanol systems. On the reduction of health and environmental impacts, it was found that acidification, human toxicity and ecological toxicity impacts occurring during harvesting and processing of

biomass were more unfavourable than favourable for bio-ethanol case studies that were investigated.

Bringing the maize to ethanol conversion into the South African context, general concerns associated with energy requirements have been raised (Mayet, 2006). Research implies that bio-ethanol produced from maize would require enormous government assistance and subsidies, for the industry to be viable, as discussed above. It is argued also that the subsidies could be allocated more appropriately to other pressing priorities in South Africa (Mayet, 2006).

A couple of emerging biomass-to-energy technologies are discussed in the next sub-section.



### 2.2.3 Novel bioenergy conversion technologies

There is a large number of emerging biomass to energy technologies, that promise either increased efficiencies in the main conversion step or that will complement other existing bio-energy technologies by removing difficulties or lowering costs at critical points in the supply chain. Two relatively new inventions are presented below to show what might be possible in the future. These technologies are the carbon conversion fuel cell and aqueous phase reforming (APR).

#### 2.2.3.1 Carbon conversion fuel cell for electricity production

A fuel cell is an electrochemical device that converts a fuel's chemical energy directly to electrical energy whilst oxidising the fuel. Whilst the principles of fuel cells have been known for about 150 years, and many fuel cell variations have been introduced over the decades, innovations have been numerous in the past decade. The most promising carbon conversion fuel cell was introduced by John Cooper and his colleagues at the Lawrence Livermore National Laboratories at the University of California in August 2002 (Cooper et. al., 2001). Their technology is a hybrid fuel cell combining direct carbon conversion and high temperature hydrogen fuel cell. The hybrid power generation system for generating electrical power from hydrocarbonaceous fuel (e.g. biomass, coal methane etc.) comprising of a pyrolysis unit for pyrolysing the fuel into carbon and hydrogen, a direct conversion fuel cell for

converting carbon into electrical power and a solid oxide fuel cell for converting hydrogen into electrical power uses very small carbon particles, whether obtained from biomass or fossil fuel, directly into electricity without traditional equipment such as steam reforming reactors, turbines and boilers.

Their direct carbon conversion fuel cell generates the electric power from the electrochemical reaction of carbon and atmospheric air. It comprises of a housing that contains a cathode and anode. A slurry, paste or wetted aggregation, consisting of carbon (extremely small particles in the range 10-1000 nanometres) immersed in molten- salt- electrolyte is introduced into the cell housing. The molten- salt- electrolyte consists of a mixture of molten alkali carbonates such as $Li_2CO_3$, $K_2CO_3$, and Na2CO3. The molten salt electrolyte provides a continuous electrolyte of carbon between the porous nickel plate anode current collector and the porous nickel plate cathode. A inert ceramic separator saturated with the molten salt is located between the anode and the cathode. Atmospheric oxygen is also fed into the reactor. The reaction takes place at temperature ranges of 750-800 $^0$C. Carbon particles react with carbonate ions to form carbon dioxide and electrons, the free electrons are delivered from the anode to an external circuit which is connected to the external motor. At the cathode oxygen, carbon dioxide and electrons from the anode react to form carbonate ions. The equations are outlined below:

Anodic half–reaction: $C + 2CO_3^{2-} \longrightarrow 3CO_2 + 4e^-$

Cathode half-reaction: $O_2 + 3CO_2 + 4e^- \longrightarrow 2CO_3^{2-}$

Overall reaction: $C + O_2 \longrightarrow CO_2$

The pure carbon dioxide ($CO_2$) product can potentially be sequestered in an underground reservoir or used to displace underground deposits of oil and gas, (Cooper, 2001).

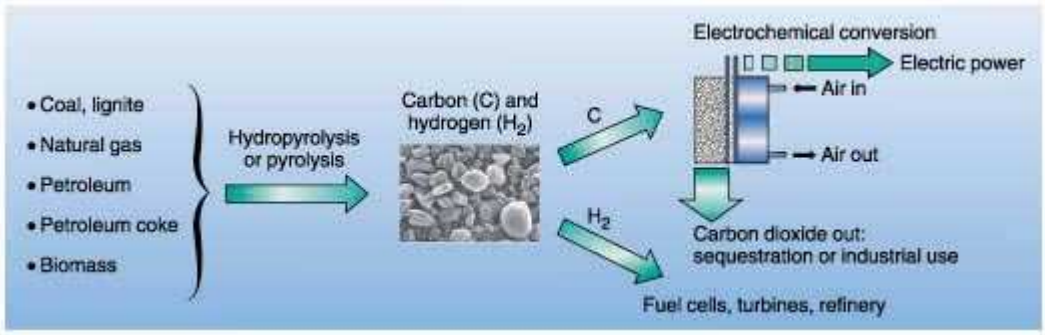


**Figure 2.2: Summary of the carbon conversion fuel cell process**
(Cooper, 2001)

### 2.2.3.2 APR for hydrogen by utilising sugar solutions

Aqueous phase reforming was introduced in 2002 (Cortright *et al.*, 2002) as a novel process route to generate hydrogen as a value-added product from aqueous phase hydrocarbons found in waste water from the food processing industry (e.g. beer brewery waste water, sugar processing, impure glycerol from biodiesel plants) and potentially also from agricultural crops such as wheat and corn.

The APR reaction proceeds through carbon monoxide as an intermediate, as shown in the set of equations below for glucose: The first reaction is the reforming reaction, the second one, the water-gas shift. The third equation is the overall APR equation. In APR carbohydrates are converted with water in aqueous phase over the appropriate heterogeneous catalyst at temperatures near 500K and moderate pressures (typically 15-50bar), where hydrogen rich effluent can be purified (Shabaker *et al.*, 2005)

$$C_6H_{12}O_{6(l)} \longrightarrow 6CO_{(g)} + 6H_{2(g)}$$

$$CO_{(g)} + H_2O_{(l)} \longrightarrow CO_{2(g)} + H_{2\,(g)}$$

$$C_6H_{12}O_{6(l)} + 6H_2O_{(l)} \longrightarrow 6CO_{2(g)} + 12H_{2(g)}$$

## *2.3 Review of Aqueous Phase Reforming (APR)*

This section discusses the key features of the APR process that favour the production of hydrogen as opposed to other competing reactions such as alkanes

and undesired aldehydes that are likely to take place at the conditions under which aqueous phase reforming (APR) can take place in.

### 2.3.1 Thermodynamic and kinetic considerations

In contrast to alkane reforming which is favourable only at high temperatures, reforming of oxygenated hydrocarbons to form CO and $H_2$ is thermodymically favourable at lower temperatures of about 400-500 K (Shabaker *et al.*, 2003). The successive water gas-shift reaction that it is necessary to convert carbon monoxide generated by the reforming reaction to carbon dioxide is also favourable at lower temperatures. Also, energy calculations indicate that the activation energy needed to break C-C bond in the oxygenated hydrocarbons is lower than that of the alkanes, indicating that C-C cleavage is easier in oxygenated hydrocarbons than in alkanes as shown in Figure 2.4 below. These results suggest that it is possible to design a process in which oxygenated hydrocarbons can be converted to $H_2$ and $CO_2$ in a single step reaction where both the reforming and water-gas shift occur at low temperature (Cortright *et al.*, 2002). Although the more volatile oxygenates such as methanol, glycerol and ethylene glycol can be processed both in vapour and liquid phase, the less volatile substances such as glucose under vapour conditions require higher temperature reforming, followed by low temperature water-shift gas, thus averting from the advantages of using a single reactor.

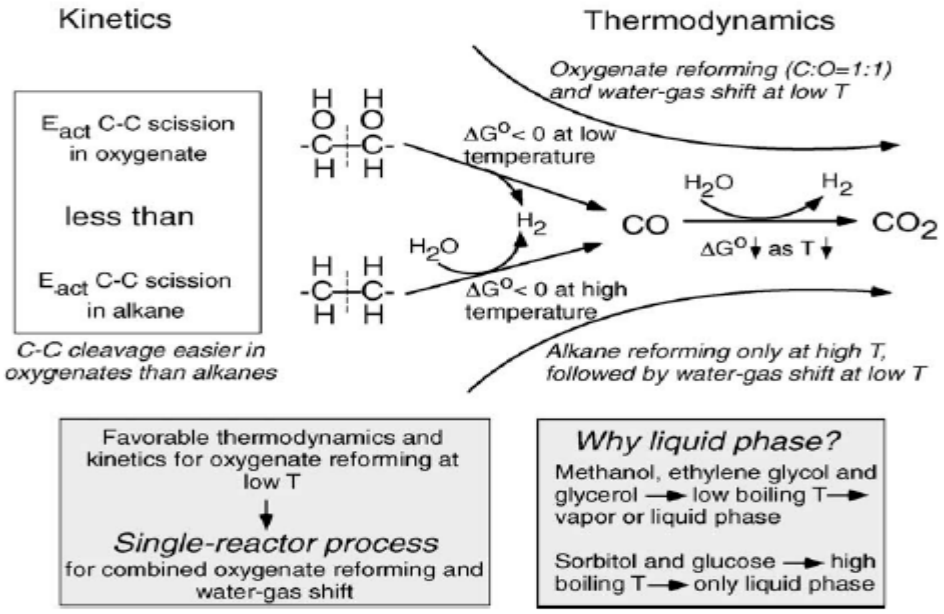


**Figure 2.3: Thermodynamic and kinetic considerations which form a basis for APR (Davda *et al.*, 2005)**

### *Selectivity*

Figure 2.5 below shows the conditions for the production of hydrogen, it also shows the process that may lead to the selective production of alkanes if desired, for the following factors: metal (catalyst), support, nature of solution and feed. This production of alkanes is suggested as an alternative route for utilising oxygenated hydrocarbons before the utilisation of fuel cells kicks off.

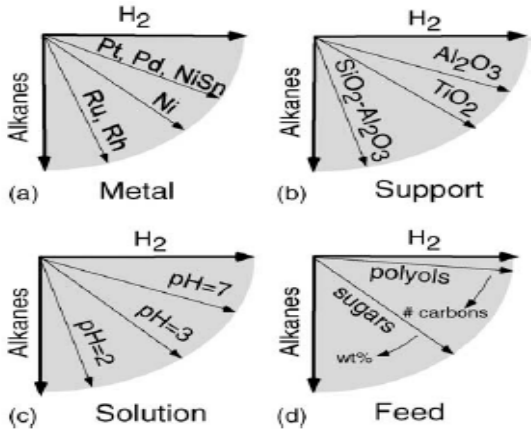


**Figure 2.4: Factors affecting selectivity of aqueous phase reforming (Davda *et al*., 2005)**



### *Metals*

The following metals were investigated by Davda *et al*. (2005); Pt, Pd, Ni-Sn, Ni, Ru and Rh. Figure 2.4a suggests that Pt, Pd and Ni-Sn alloys show high selectivity for hydrogen production and very low selectivity for the alkanes production. However, Ni metal tends to favour the production of alkanes, and it is also known for its deactivation with time. This is thought to be the result of the sintering of metal particles. Ru and Rh are very active for the production of alkanes at the same reaction conditions.

### *Supports*

Tests also showed metal supports to be an important factor to the selectivity of the APR process as seen in Figure 2.4b. It was observed that basic/neutral supports favour hydrogen production. The more acidic supports however, (e.g. silica-alumina) favour the production of alkanes. Supports which have medium acidity, as seen for the titania-based catalysts fall within the spectrum of extremes (Davda *et al*., 2005).

***Solution Conditions***

Depending on the nature of the intermediate of by-product compounds formed in the reactor, the aqueous solution in contact with the catalyst can be acidic, neutral or basic. Acidic solution (pH =2-4) favours the selectivity of alkanes. In contrast neutral and basic solutions lead to high hydrogen selectivities and low alkane selectivities as shown in figure 2.4c (Dumesic *et al.*, 2004).

***Feed type***

The type of feed has a strong influence on the selectivity of the APR reactions. Generally polyols (e.g. sorbitol, hydrogenated glucose) have higher hydrogen selectivity than sugars (e.g. glucose). Within the family of polyols, hydrogen selectivity decreases with the increasing carbon number of the feed. The reason is said to be that undesired consuming reactions increases accordingly. A higher feed concentration of glucose also leads to lower selectivities. For example, as the glucose feed concentration increases from 1 to 10 wt.%, the alkane selectivity increases from 30% to 50%, the hydrogen selectivity then decreases accordingly (Davda *et al.*, 2005). The change is attributed to undesired homogenous decomposition reaction associated with sugars. These feed effects are summarised in figure 2.4d.



## 2.3.2 Attaining a low concentration of CO in the product

Low CO levels in the product gas can be obtained at the reaction conditions by harnessing the concept of 'ultra-shift'. Figure 2.5 below outlines this concept of driving the CO levels to as low as possible. Based on the water-shift equilibrium, partial pressure of CO ($P_{CO}$) in the reactor is proportional to that of hydrogen ($P_{H2}$). $P_{H2}$ decreases as the partial pressure of water ($P_{water}$) in the system approaches system pressure ($P_{total}$). Therefore to lower the partial pressure of CO in the reactor, the hydrogen pressure should be decreased by increasing the water pressure in the system. This is the point where ultra shift process comes into play, where the water pressure is increased either by reducing the system pressure in an isothermal reactor or increasing the temperature of the upper shift-zone of the isobaric reactor. For an example if the shift temperature is maintained at a reforming temperature of 498K, the concentration of CO increases as the system pressure is increased. However if

the shift temperatures are increased such that the majority of liquid water vaporises, the CO concentration decreases to even as low as 100ppm (Davda *et al.*, 2005). Therefore the addition of the ultra-shift zone to the reforming reactor leads to low CO levels while allowing for processing of non-volatile glucose in the lower-aqueous phase reformer.

When the effluent from the reactor is cooled to condense liquid water, then the pressure of the non-condensable gases increases and approaches the system's pressure. This process of ultra-shift involving initial vaporisation followed by condensation of water, thus leads to a desirable fuel cell grade $H_2$ with low CO concentrations.

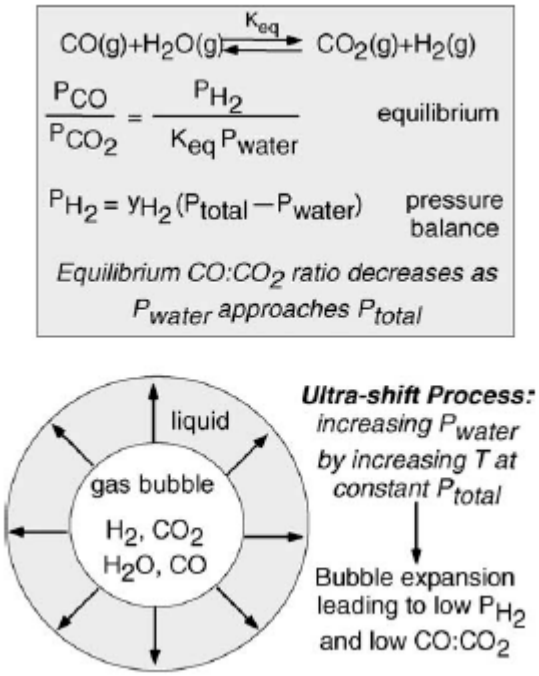


**Figure 2.5: Concept of the ultra-shift process for obtaining low CO levels in the product gas (Davda *et al.*, 2005)**

### 2.3.3 A reactor system for concentrated glucose feeds

It was established that APR has poor selectivity for highly concentrated glucose feedstocks – the most likely intermediate deriving from hydrolysis of starches or lingo-cellulosic feedstocks. These limitations are addressed by the dual-reactor process concept as summarised in Figure 2.6 below. One of the important aspects is that the hydrogen selectivity increases when higher concentration feeds are used. This limitation is said to be specific to glucose feedstocks and not sugar-alcohol, for

example sorbitol is said not suffer this restriction (Davda *et al.*, 2005). Glucose can undergo hydrogenation (Using $H_2$ from reforming or supplied externally) to form sorbitol, which can then undergo reforming on the catalyst surface to form desired $H_2$ and $CO_2$. The hydrogenation reactor is operated at low temperatures of about 370K. At low vapour pressure of water corresponding to this hydrogenation temperature, the partial pressure of hydrogen is high, and favourable for the conversion of glucose to sorbitol. The relative rates of different reactions involved in glucose processing thus indicate that for efficient extraction of hydrogen from glucose feedstocks, it is necessary to utilise the initial hydrogenation reactor that converts glucose into sorbitol, followed by the reforming reactor that produces hydrogen with high selectivities (Davda *et al.*, 2005).

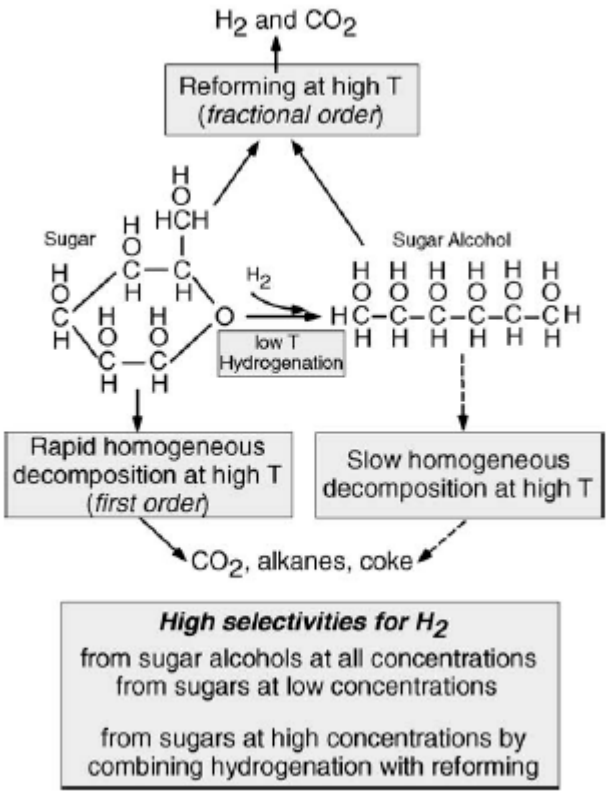


**Figure 2.6: Basis for dual-reactor system employed in the processing of concentrated glucose (Davda *et al.*, 2005)**

## *2.4 Life Cycle Assessment in technology assessment*

### 2.4.1 Overview of Life Cycle Assessment (LCA)

The environmental performance of products and processes has become a key issue in many companies, and many have found it useful to move beyond compliance, using pollution prevention strategies and environmental management systems to improve their environmental performances. One environmental assessment tool used in this context is Life Cycle Assessment, LCA, which considers the whole life cycle of the product or the process to be improved. By including the impacts through the product's life cycle, LCA offers a comprehensive view of the environmental aspects associated with a product or process and a true picture of the environmental trade-offs in product and process selection (Curran, 2006). This standardised and quoted tool used to measure sustainability has been chosen as a tool for the present study. However, its operational hierarchy and generic methodology will not be discussed here, as there is much open literature and web access on the methodology and hierarchy, some of the useful sources are Curran *et. al.* 2006; http://www.epa.gov/ORD/NRMRL/lcaccess.

### 2.4.2 Different types of LCA

Several efforts have been made to classify LCA (Tillman, 2000); in particular two categories have been highlighted. This section distinguishes between these two types of LCA, attributional and consequential. These terms were adopted in 2001 at a workshop on LCI electricity data in Cincinnati (Curran, 2006). Several authors have similar distinctions of the two types of LCA, although they employ different terms, (Weidema, 1993; Baumann, 1995).

#### 2.4.2.1 Attributional LCA

This type of LCA aims at mapping the environmental impacts that a product can be made accountable for, so it can be called accounting, descriptive, retrospective or attributional (Sanden and Kalstrom, 2007). This approach recommends tracing all flows from cradle to grave and that everything should be included and accounted for, whether relevant or not. Ideally attributional LCA should include average data of each of the units in the life cycle (Ekvall, 2005). The criteria as to whether a unit process maybe omitted is not based on whether the flows are negligible i.e. they are not based on its relevance to a potential change in a system that is being designed,

which is viewed by some as a drawback (Tillman, 2000). Most of the older studies in LCA are said to resemble this type of LCA (Ekvall, 2005).

### 2.4.2.2 Consequential LCA

This type of LCA aims at describing consequences of change, so it is called change-oriented, prospective, or consequential LCA. This perspective is assumed to be forward looking (Sanden and Kalstrom, 2007). Prospective LCA investigates the likely environmental consequences for a decision that has been proposed as a more appropriate mode i.e. of the relevant physical flows to and from the technosphere. This type of LCI model includes unit processes that are significantly affected irrespective to whether they are within the life cycle (Ekvall, 2005). Ideally, it should include marginal data on bulk production in the background system, and allocation is usually avoided by means of system expansion (Ekvall, 1999 & 2005). However, Ekvall (2005) concludes that consequential LCA has limitations, among them; the lack in completeness, accuracy and relevance. Concerning completeness, he argues that full consequences of change can not be fully described for at least two reasons, i) the future is inherently uncertain and ii) there are large data gaps of various types. Certain decision-makers can also be more interested in knowledge on environmental properties of the system (generated by the retrospective LCA) than in knowledge of the effects of change within the life cycle (generated by the prospective LCA), rendering this type of LCA irrelevant to them.

**Table 2.1: A summary of relevance of retrospective and prospective perspective to different types of LCA applications**

| Types of LCA | Attributional | Consequential |
|---|---|---|
| Applications | Learning<br>Application of improvement possibilities<br>Market claims | Changes in:<br>Product design<br>Process design<br>Regulatory measures aiming for change |

From a strategic technology choice, some authors find it useful to suggest one more distinction in retrospective and prospective LCAs: between product and technology, where the former seeks to investigate the impact of a specific product, plant or production process, while the latter is an assessment of more general technology. Therefore, the retrospective and prospective technology LCAs can be used to support decisions on strategic technology choice (Sanden and Kalstrom, 2007).

## *2.5 Recent LCA application to bioenergy systems*

This section reviews key studies isolated from the literature which are relevant to the research presented here. Many investigations have been carried out in the field of bioenergy systems LCA in recent years. This section reviews recent evaluations only i.e. those that were compiled approximately in the past four years, most LCA studies prior to that have already been reviewed elsewhere (Curran & von Blottnitz, 2007). This section comprises of objectives for carrying out LCAs, followed by LCA of cropping systems for the production of biomass utilised for biofuel production, following which LCA for various energy products will be explored. This section will then be concluded with a discussion of some of challenges that are still facing the sustainability of bioenergy systems. Table 2.2 below presents a summary of selected literature that will be discussed in the subsequent subsections.

**Table 2.2: A summary of types of LCA and LCIA methods from the selected studies**

| Source | Type of LCA | LCIA method | Impact Categories |
|---|---|---|---|
| Kim and Dale (2005a) | Product attributional | EPA-TRACI | Use of non renewable resources, Global warming, acidification and eutrophication |
| Kim and Dale (2005b) | Product attributional and consequential | EPA-TRACI | Use of non renewable resources, Global warming |
| Bernesson *et. al.* (2003) | Technological attributional | - | Photochemical oxidation potential, global warming, acidification and eutrophication |
| Zah *et. al.* (2007) | Product attributional | Eco-indicator 99, Points UB 06 | Global warming, acidification and eutrophication |
| Eriksson *et. al.* (2007) | Technological consequential | CML 2000, Ecoindicator 99, Eco-Tax 02 and EPS 2000 | Use of natural resources, global warming, toxic emissions |

### 2.5.1 Objectives for performing LCAs for bioenergy systems

Different objectives for performing LCAs were identified from the selected literature on bioenergy systems. For Zah *et al.*, (2007) whose study involved the evaluation of the environmental impact of the entire production chain of the fuels made from biomass used in Switzerland; their main objective was tied to political decisions which play a major role in structuring of biofuel policies.

Similarly, Eriksson *et al.* (2007) carried out a life cycle assessment whose main objective was to contribute to policy-making in the energy sector in Sweden. The LCA entailed comparison of environmental consequences of district-heating production from waste and competing fuels in Sweden. Their study also includes how the environmental impacts are avoided by the displaced electricity production when power is produced combined with heat production.

The objective of another study was to investigate the environmental impact which the choice of cropping systems have for producing biofuels: Kim and Dale (2005b) carried out such a study for different cropping systems emphasising corn and soybean production for bioethanol and biodiesel production. Bernesson *et. al.* (2004) carried out a study that explored the implications associated with the choice of scale of the plant for biofuel production.

Yet another objective identified was to analyse the environmental superiority of either new bio-energy technologies or renewable fuels before they enter into the market by comparing competing options. Pehnt (2006) investigates the dynamic approach towards LCA of renewable energy technologies, for instance he explores the improvement potential of the competing technologies e.g. due to process and system innovation, while Weisser (2006) addresses the same issue but from electric supply technologies perspective (fossil and renewable).

Finally, one objective that was deduced from selected literature is the implications of displacing the gasoline in spark ignition engine (SI) by biofuels such as bioethanol, bio-ethyl tertiary butyl ether (bioETBE) and biodiesel. Malca and Freire (2006) made an analysis of Life Cycle energy assessment of bioethanol and bioETBE by proposing a novel indicator aiming at characterising renewability of the proposed bioenergy

sources – the energy renewability efficiency, which measures the fraction of final fuel energy obtained from renewable sources.

This sub-section focussed on reasons behind the undertaking of LCA studies on the bioenergy systems have been undertaken in the bioenergy. The next sub-section identifies studies that are most relevant to the study at hand and explore methods of analysis used.

## 2.5.2 Methods used in the bioenergy LCAs

This section seeks to highlight methods used in life cycle assessment of bioenergy systems from the selected studies. First, the types of LCA used will be classified in the light of the classifications already introduced in section 1.4. Secondly, the types of LCIA and the impact categories investigated in the individual studies will be looked into.

### 2.5.2.1 Types LCA used in the selected literature

The types of LCA employed in the individual life cycle assessments depended on the aims and objectives of the studies. In their life cycle assessment of fuels for district heating, Eriksson *et. al*. (2007) objective was to compare the environmental consequences of district heat production from waste compared to other fuels used in Sweden. The nature of the study is technological consequential in a sense that technologies that produce biofuels are used in the analysis and that data used reflect marginal electricity production.

Kim and Dale (2005b) on the other hand carried a life cycle assessment of different cropping systems emphasising corn and soy bean production with an assumptions that biomass is used solely for the production of biofuels. Their assessment reflects a combination of the two types of LCAs, attributional and consequential because the cropping system scenarios investigate both the current situation and future scenarios which show what could be possible in the future. Since then the scenarios investigated the production systems not the product a further classification would categorise the types of LCA used as both technological attributional and consequential.

In another study Kim and Dale (2006) carried out an attributional LCA in a comparative study where the environmental performance of two ethanol transport applications, E10 and E85, where E10 is a mixture of 10% ethanol and 90% gasoline, while E85 is a mixture of 85% ethanol and 15% gasoline. The nature of the LCA is product attributional since both the products are analysed from cradle to grave and are produced by well developed technologies. Bernesson *et al*. (2004) also used a technological attributional LCA to compare the environmental performance of large, medium and small scale production of rape methyl ester (RME) under Swedish conditions, where the data used represented averages of the existing technologies.

Yet another study (Zah *et al*., 2007) carried out product attributional LCA, where the life cycle assessment for the entire production chain of fuels made of biomass was in Switzerland were investigated. The comparison carried out in this study provides a holistic comparison of the environmental performance of biofuels (bioethanol, biodiesel, biomethanol and biogas) from cradle to grave.

#### 2.5.2.2 Methods of LCIA used and impact categories investigated

Aims and objectives of a life cycle assessment contribute a great deal to the choice of impact categories and life cycle impact assessment (LCIA) method used in the analysis of the inventory results. On the other hand the type of LCA software employed depends on either preference or availability. This sub-section reviews the LCIA methods and impact categories employed in the studies and the rationale behind the choices.

In their LCA of fuels for district heating, Eriksson *et. al*. (2007) used the following impact methods: CML 2000 as a characterisation method, and EcoTax 02, Eco-indicator 99 and EPS 2000 as weighting methods. Although previous studies (Finnveden *et al*., 2005) have indicated that the most significant impact categories in waste management may be the use of natural resources, global warming potential and toxic emissions, they opted to use the following impact categories: the use of energy, global warming potential and the total weighted product. The type LCA software employed in the study is SimaPro 5. The following conclusions were reached; CHP has environmental benefit compared to only DH in terms of the selected impact categories. The use of biofuels as one of the other fuels that was

compared with the waste has more environmental benefits compared to other fuels such as natural gas.

In the LCA of different cropping systems for maize and soybean production Kim and Dale (2005b) made the assumption that biomass from the cropping systems were used solely to producing biofuels. The basis for comparison was taken to be 1 hectare of arable land used producing biomass for biofuels to compare the environmental performance of the different cropping system. The potential environmental impacts were estimated by characterisation factors given by the Tools for the Reduction and Assessment of Chemical and other Environmental Impacts (TRACI) model, proposed by the United States Environmental Protection Agency (EPA-TRACI).

The following environmental impacts were deemed relevant to the study at hand: non-renewable energy consumption, global warming potential, acidification and eutrophication. Some of the key results that stemmed out of the study were as follows: when biomass from cropping systems is utilised for biofuel production, all the cropping systems studied offer environmental benefits in terms of use of non-renewable energy consumption and global warming potential. Thus utilising biomass for biofuel will reduce dependence on fossil fuels and reduce green house emissions. It was concluded however that unless additional measures such as planting cover crops were taken, utilisation of biomass for biofuels will also tend to increase the impact of acidification and eutrophication primarily because of the large nitrogen (or phosphorus) related environmental burdens that are released from soil during cultivation.

Kim and Dale (2006) carried out a comparative LCA which investigated the environmental performances of the two ethanol applications (E10 and E85). Two types of functional units were considered in the study, an ethanol production oriented perspective and the travelling distance oriented perspective. The ethanol production-oriented functional perspective reflects that the ethanol fuel supply (arable land or quantity of biomass used in ethanol fuel) is constrained, while the travelling distance-oriented functional unit implies that the ethanol fuel supply is unlimited.

The potential impact categories represented here are natural resources used, non-renewable energy, global warming potential, acidification and eutrophication. The characterisation factors used are adopted from the TRACI model. Key results that can be drawn from this study are that the functional unit affects the final results significantly. Thus it is essential that the functional unit reflects as nearly as possible the situation associated with the product system. Considering the fact that ethanol is not readily accessible, the E10 fuel offers the better environmental performance in natural resources used, non renewable energy and global warming potential unless the fuel economy of an E85-fuelled vehicle is close to that of an E10-fuelled vehicle.

The study on a limited life cycle assessment carried out by Bernesson *et. al.* (2004) compared the environmental performances of large, medium and small scale production of rape methyl esters under the Swedish conditions. The limited LCA undertaken here include air emissions and energy requirements. The emissions were classified in the following environmental impact categories: Global Warming Potential (GWP), Acidification Potential (AP) Eutrophication Potential (EP) and Photochemical Oxidant Creation Potential (POCP). The LCIA method used in the study was not been explicitly stated. It was concluded from the study that all the energy requirements and the environmental impacts, according to the impact categories mentioned above, are very similar.

Zah *et al.*, (2007) in their study on the environmental assessment of biofuels in Switzerland used two Life Cycle Impact Assessment methods. One was the Swiss method of ecological scarcity (Environmental Impact Points UB 06) which evaluates the difference between the environmental impacts and legal limits. The other method is the European Eco-indicator 99 methods. This study like all the previous studies discussed above was classified in the following environmental impact categories: Global Warming Potential (GWP), Acidification Potential (AP) and Eutrophication. They concluded that not all biofuels reduced the environmental impacts compared to fossil fuels; however the environmental impacts of biofuels unlike those of fossil fuels can be reduced a lot by appropriate measures.

### 2.5.3 Comparison of biomass for fuel versus power generation

Biomass can be utilised to produce biofuels for transport purposes, but it can also be used for heat and power generation. A study under undertaken by Crozoen (2005) compared the two options of biofuels and power generation up to 2010. The analysis investigated the two options on a basis of the same cropland area for the power and for the transport fuel scenarios and the energy output for both the systems. Three indicators were used to compare the two scenarios, the greenhouse gas emissions, cropland requirements and the costs. Comparisons based on the cropland for the two scenarios showed that energy crops are more effective in reducing carbon dioxide emissions if they are burned in a coal fired station via indirect combustion or co-firing with syngas in a CHP configuration. Comparisons based on the same displacement of the fossil fuels also show that extra costs are lower for the power generation scenario.

Zah *et al.* (2007) explored a similar notion to that of CE for utilising biomass to produce transport fuel and power generation. In their electricity analysis, however, they do not only focus on crops that are grown specifically for heat and power generation (e.g. wood), they investigate also the impacts of generating heat and power from energy carriers such as biogas and transport fuels such as bioethanol. In their analysis they found that not all the utilisation possibilities are equally advantageous from a life cycle perspective because they involve certain percentages of conventional energy carriers such as fossil fuels. They investigated which of the energetic utilisation is most environmentally friendly between transport fuel route and heat and power generation utilisation. This was carried out by calculating the net utility for various biogenic carriers using the following formula:

**Net utility** = environmental impact avoided by using substitutes for fossil energy carrier – environmental impact produced by using the biogenic energy carrier.

The functional unit was a certain quantity of a biogenic energy carrier (for instance 1 litre of ethanol) which yielded a certain quantity of energy to be used as heat, electric power or transport. The results were compared on a basis of Global Warming Potential using Eco-indicator '99. From the Life cycle assessments it was

concluded that using the variations tested as substitutes for traditional energy carriers will bring positive results as regards the GHG emissions, and thus less global warming potential, it does not however produce positive results for environmental LCA in all cases. For instance whey-derived ethanol showed better results in terms of GHG emissions when used in cogeneration (CHP) compared to when it is used as transport fuel however it performed poorly in other impact categories studied.

### 2.5.4 Key findings from the selected literature

The following findings emerge from the reviewed studies on recent LCAs of bioenergy systems:

***LCA classification***

The type of LCA used is largely a consequence of the objectives of the study; it was observed that a study does not have to be restricted to one type of LCA and that a combination of LCA types as classified above can be employed. Most of the previous studies focussed on attributional LCA, which merely accounts for environmental impacts of a process or product, an observation reflective of the claim that most of the older LCA studies are attributional Ekvall (2005). Consequential LCA is slowly gaining momentum in recent years, where future scenarios are explored mainly to assist with strategies on sustainable policies.

***Functional unit selection***

The importance of selecting a functional unit that it is representative of the situation at hand is crucial. Different functional units employed for the same product systems give very different results as seen from a study by Kim and Dale (2005a).

***Methods used in LCA analysis***

The types of LCA analysis tools differ for different studies, however impact categories used in individual LCAs are very similar and include global warming potential, acidification, and eutrophication as summarised in Table 2.2 above. In addition to the impact categories there is further exploration on the use of resources and replacement of non-renewable resources. Methods of LCIA used differ according to the objective of the study; while most of the studies use only the characterisation

method to analyse inventory results, others use weighting in addition to characterisation.

***The use of CHP in biofuel systems***

The use of CHP in the biofuel arena gives an overall improvement in the environmental performance when energy crops or/and energy carriers such as ethanol are used to generate heat and power compared to utilising the same raw material for power generation only (Crozoen, 2005; Zah *et al.*, 2007).

### 2.5.5 Challenges that face LCA in bioenergy systems

It is recognised that the methodology of LCA focuses on the environmental impacts of materials and energy flows, and that it does not address the other sustainability dimensions (economic and social) with the same rigour, despite much work on Life Cycle Costing on the one hand, and on inclusion of social concerns on the other.

One other important environmental impact of biofuels production which LCA covers poorly is that of land use. Although the importance of land use evaluation has recently been recognised in LCA there is still a considerable lack of definition concerning the parameters that need to be considered. Anton *et al.* (2005) reviewed different methods proposed for assessing environmental impact of the land use. They found that most of the methodologies that have been proposed use a number of indicators that are largely dependent on the availability of data. The general trend in the comparison of conventional agricultural land use with integrated agricultural land use show little difference in terms of vascular plants and very few differences concerning the occupation of the soil.



## *2.6 Summary of the literature review*

In this chapter, literature relevant to the study at hand was reviewed. The key conclusions are as follows:

- The South African government has come up with strategies and policies that address issues associated with biofuel and hydrogen production and use in the economy. It has been realised however that although South Africa has

limited arable land for farming, there is available land mainly in the former homelands that has not be utilised to the full potential that could be used for bio-fuel crops.

- It essential that bioenergy conversion systems with better efficiencies be explored in South Africa for the government to achieve the set targets and ambitions on renewable energy. There is a need to look to up-coming technologies (the so-called second generation) for better efficiencies, as most of the established ones suffer from low yields or efficiencies. A second generation biofuel technology called Aqueous Phase Reforming (APR) could have potential application in South Africa because of its claimed ability to utilise any sugar solutions with higher efficiencies. However the environmental merit of this technology is yet to be tested.

- Life cycle assessment has been recognised as a suitable tool for the study at hand which investigates the merit of a second generation biofuel technology in a particular context. From a review of recent LCA studies on biofuels it was concluded that methods used depended on the objectives, while the impact categories employed were found to be largely uniform.

- The sustainability of the maize to ethanol conversion route was investigated as a foundation onto which the comparison with the APR will be based, since they are able to utilise the same sugar streams. Most literature concurs with the fact that this route suffers from low energy yields compared to other feedstock such as sugar cane for the production of ethanol.

- The use of Combined Heat and Power was found to have better overall environmental impacts if power is to be generated using either energy crops or secondary energy carriers such as ethanol.

# 3 Methodology

The methodology developed to achieve the objectives of this dissertation (as stated in chapter 1) is based on the formulation and testing of hypotheses. A first hypothesis was stated in chapter 1 as follows:

1. Using energy products derived from maize for electricity generation as opposed to vehicle fuel is environmentally attractive in South Africa because of the relatively high environmental impact of the coal based electricity.

Building on a key finding from the literature review on the environmental performance of bio-ethanol, and in particular of the negative consequences of high usage of coal to provide process heat for the distillation process, the following 2nd hypothesis is now proposed:

2. Where electricity is to be generated from the maize derived energy products, heat integration into the production plant by means of combined heat and power (CHP) has better energy yields and environmental benefits compared to electricity generation without heat integration.

In addition, on taking note that life cycle assessments are meant to extend to product use and not only end at the 'gate', the following 3rd hypothesis is put forward:

3. The environmental performance of both the ethanol and the hydrogen option can be improved not only by changes in production efficiency, but also by technology improvements in the product use-phase.

This chapter begins by presenting an overview of approach developed and methods used to test the hypotheses through a schematic flow diagram presented in Figure 3.1 below. Section 3.2 discusses methods used in compilation of the Life Cycle Inventory (LCI). Section 3.3 presents the methods of life cycle impact assessment (LCIA) employed in the study. Section 3.4 discusses the approach used to allow for the comparison of electric energy products with vehicle fuel products, which is followed by concluding remarks in 3.5.

## *3.1 An overview of the procedure followed*

The procedure adopted in the testing of the hypotheses required that a clear definition of the LCA and its implications be made. One of the four steps of any LCA is goal definition and scoping. This is discussed in detail in chapter 4. In broad terms the goal of the study was not only to compare the two energy products (hydrogen and ethanol) derived from maize, but also their respective use in two broad industrial-based application categories, the transport and the power generation sectors, particularly, peak power generation. A schematic diagram below gives an outline of the procedure:

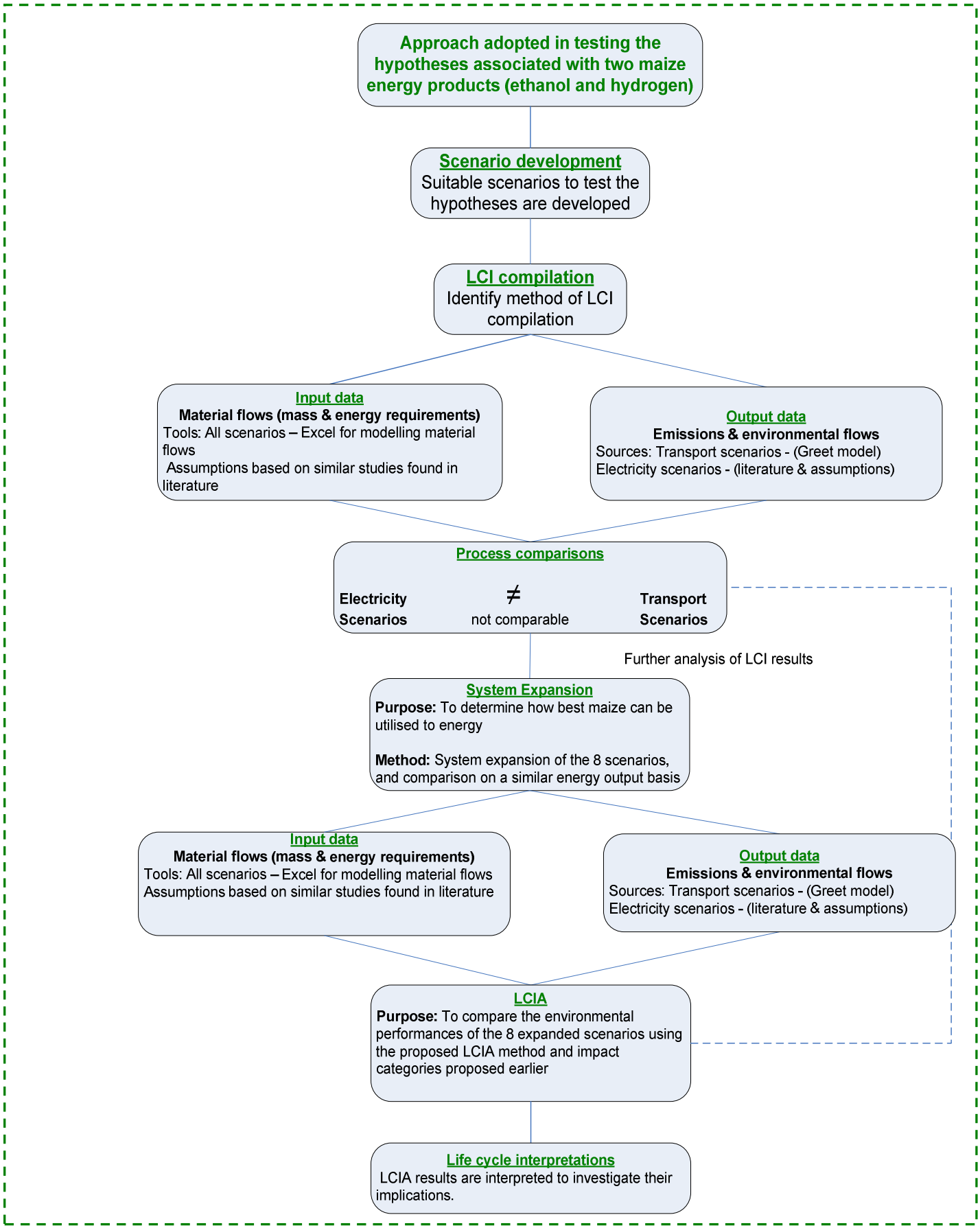


**Figure 3.1: An outline of a procedure undertaken to test the hypotheses**

## *3.2 LCI compilation procedure*

In addition to the production of bio-ethanol for use as motor fuel, seven possible future industrial applications options are proposed and evaluated in order to test the hypotheses. Two electricity generation options based on the maize energy products are proposed as alternative to vehicle fuel options to address hypothesis 1. Two more electricity scenarios that incorporate heat integration with power generation are proposed to address hypothesis 2. Transport options provide a good basis for assessing how best maize energy products could be utilised, therefore in support of the 3rd hypothesis, two additional transport options involving fuel cell technology are proposed.

Life cycle inventory (LCI) analysis is defined as a phase of life cycle assessment (LCA) that involves the compilation and quantification of input and output flows for a given product or process system. Several methods for LCI compilation have been identified, including computational approaches that include process flow diagram and matrix inversion, data gathering from industrial operations, and economic methods that utilise the Input-Output Analysis (Rebitzer *et. al.*, 2004, Suh and Huppes, 2005). Using process flow diagrams has been the most common practice among the LCA practitioners.

The process flow diagram approach was employed in the current study for the following reasons: a) its simplicity in terms of application, b) computational tool requirements are satisfied by spread-sheeting (Excel) which is readily available, c) its availability in most LCA software tools. A process flow diagram (PFD) depicts how processes that make up a product or a process system are interconnected through material and environmental flows. In this study, the LCI was compiled with the aid of Excel spreadsheets. Material balances over the process flow diagram were calculated in Excel to obtain both the material and environmental flows. The subsequent subsections will discuss procedures followed in obtaining LCI input through mass and energy balance and how the output flows were modelled. The flow diagrams over which the material balances were made are illustrated in the figures below:

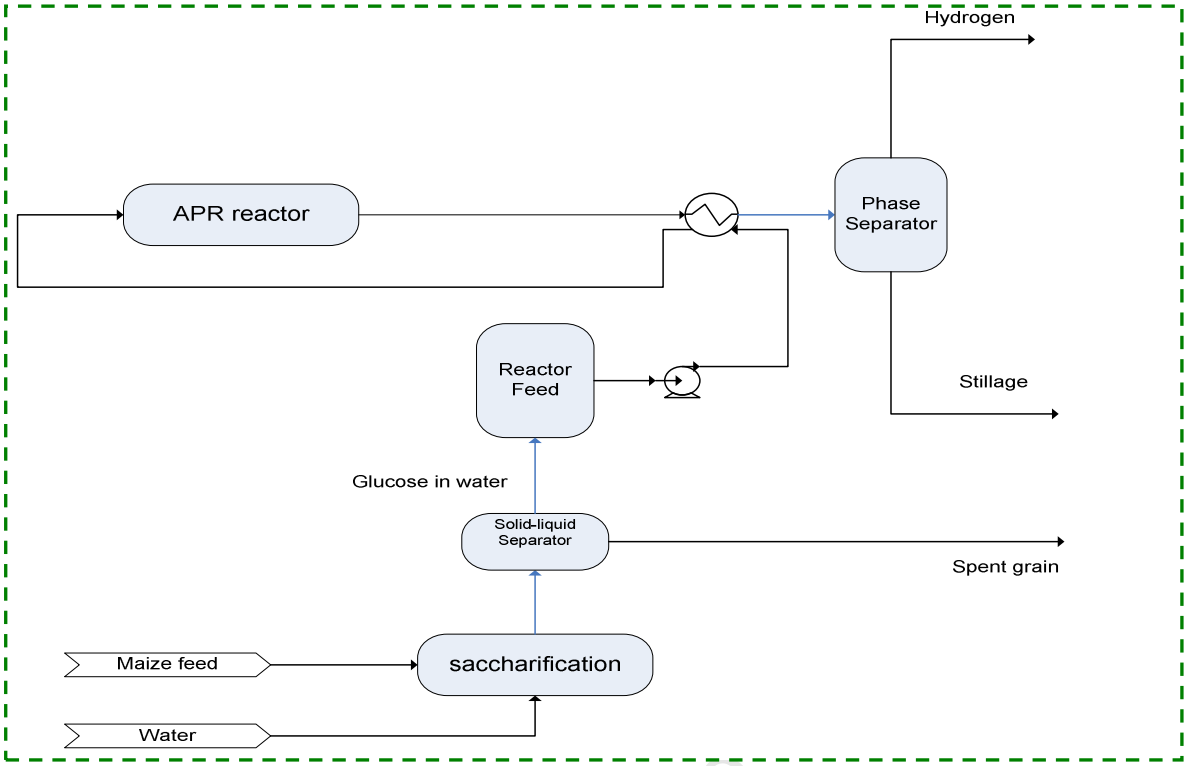


**Figure 3.2: Process flow diagram for the APR process**

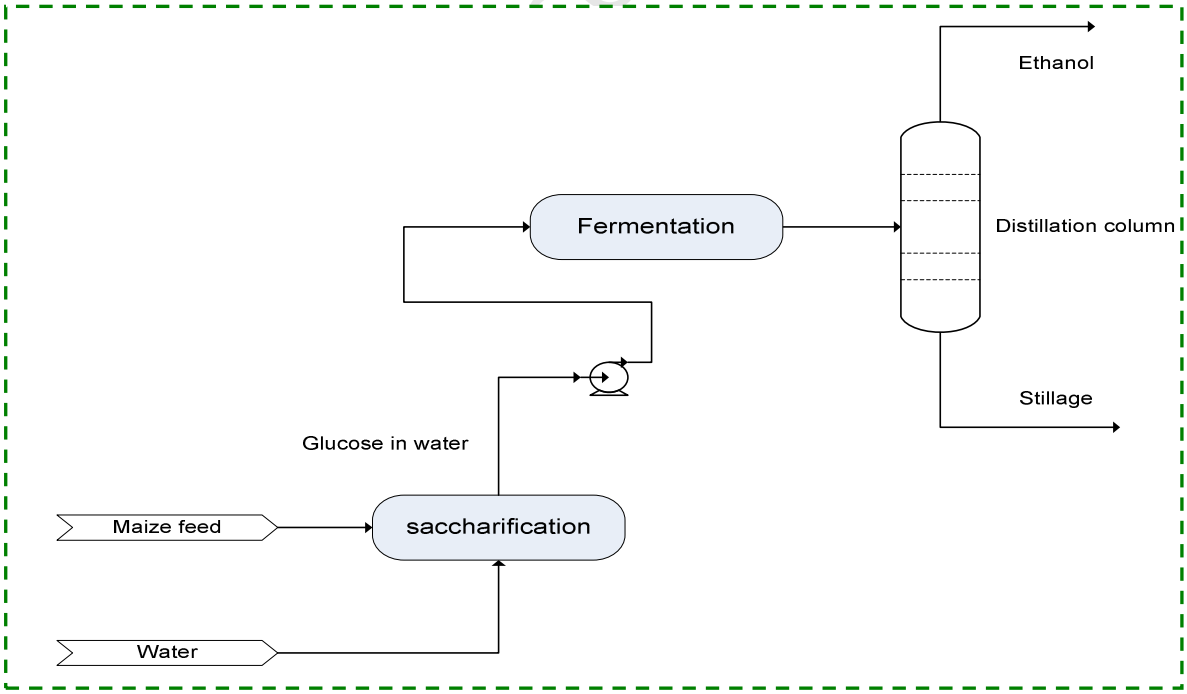


**Figure 3.3: Process flow diagram for the fermentation and distillation of ethanol**

## 3.2.1 Material and Energy Balance

### 3.2.1.1 Introduction

This subsection presents the approach followed in modelling material flows of the processes presented in Figures 3.2 and 3.3 above. The primary data used for the material balance was sourced from the Grain SA website, Department of Agriculture website and some of the open source literature. For the validation of some of the data used in the calculations, data from similar studies was compared and averaged where necessary.

### 3.2.1.2 Material balance assumptions

There were three major assumptions used in the material balance calculations:

1. The conversion of the starch-derived glucose was assumed to be the same in both the conversion systems, APR and fermentation. This is due to limited data available for a large scale APR process a result of a comparison between a technology undergoing R&D and an established fermentation process. Early literature on APR predicts that almost all the glucose in solution will be converted into hydrogen, which is also achieved in fermentation of glucose into ethanol achieving a conversion of 51 % of ethanol from maize. This also forms a good basis for comparison of the energy products as products derived from the same amounts of glucose (and hence maize and hence land).

2. The phase separation of the APR reactor product into gas and liquid streams is assumed to be 100% efficient, and that the gas stream comprises mostly of hydrogen. This is not necessarily precise because of the formation of alkanes and aldehydes in the competing reactions which can be minimised by optimising conditions that favour the selectivity of hydrogen as extensively discussed in chapter 2. Also, in the energy yields based on the product streams for both processes, ethanol and hydrogen streams were assumed to have a composition of 100%.

3. The stillage, a by-product of ethanol distillation is assumed to contain twice as much COD (chemical oxygen demand) compared to the corresponding APR liquid effluent. The ethanol that is not recovered in the distillate ends up in

the stillage and contributes a considerable amount to the overall COD (Wilkie *et al.*, 2000) hence the hydrogen liquid effluent was assumed to contain half the COD of the stillage. This assumption is crucial as it affects the results of the LCIA, especially those that are directly impacted by the COD content in effluent streams.

Through the completion of material and energy balance the following data is obtained for LCI analysis:

i. The quantities of ethanol and hydrogen produced from fermentation and distillation and APR process respectively.
ii. The process heat requirements obtained from the energy balance for the ethanol production, for validation, the energy balance calculations were compared to the literature values and were found to be in good agreement.
iii. Energy yields based on the product streams of ethanol and hydrogen.
iv. The amount of stillage (in the case of ethanol production) and water effluent in the APR process.
v. Amount of water utilised by both processes.
vi. The amount of biogenic carbon dioxide produced in the production phase.

### 3.2.1.3 Methodology

The material and balance was calculated on a basis of maize cultivated from 1 hectare of land, the functional unit of the LCA (as will be motivated in section 4.1). The yield for the 2005/06 season, reported to be 3.86 tons/hectare (www.grainsa.co.za) was used in the calculations. The starch content of the maize kernel was reported to be 70% (www.fao.org; http://www.sagl.co.za/maize_analysis.aspx), the amount of starch converted into glucose in the saccharification step is about 99% (Wilson et. al., 2004). Glucose instead of starch is used to calculate the amounts of ethanol and hydrogen produced which are further used in the energy balances and the LCI.

#### *Ethanol production material and energy analysis*

##### *Mass Balance*

The basis for the mass balance for the ethanol production was taken to be 2.67 tons/hectare of glucose derived from the 3.86 tons/hectare of maize. The amount of

water used for the process was deduced from the typical concentration of glucose in fermentation reactors of about 17.5 wt% (Ljiljana *et al.*, 2006). The quantity of water used was calculated to be 12.7 $m^3$ essential to achieve the required composition of glucose in solution. Stoichiometric ratios were used to calculate the fermentation products as presented in Appendix 2. The resulting fermentation liquid product contained 9.5 wt.% of ethanol, which is in agreement with most the fermentation product streams beyond which the yeast will begin to be inactive (Krishman *et al.*, 2000). The amount of biogenic carbon dioxide produced is 1.28 tons, and the ethanol product was calculated to be 1.34 tons. The distillation column was assumed to be operating at maximum efficiency and that the ethanol recovery of 95 % into the distillate (Ljiljana *et al.*, 2006) was achieved resulting in 1.3 tons of ethanol produced with a distillate composition of 96%, water making up the remainder. The amount of spent grain, the non-starch, high nutrient maize kernels, water and some unrecovered ethanol forms a liquid effluent referred to as stillage that exits the bottoms of the distillation column. The stillage comprises mostly of process water in the effluent at 12.6 $m^3$ and non-starch maize kernels that amount to 1.16 tons, the unconverted glucose, 54 kg, and the un-recovered ethanol, 68 kg .

### *Energy Balance*

The purpose of an energy balance is to estimate the energy requirements for the process, one of the essential data for LCI compilation. The energy balance was carried out over the fermentation unit and a distillation column in accordance with the goal and scope of the LCA. A first order energy balance was carried out over the fermentation reactor while ASPEN simulation software was employed for modelling the energy requirements of the distillation column.

In calculating the energy requirements of a fermentation reactor, mass balance results and constant heat capacities (Cp) values for water and ethanol were employed because of a small temperature difference between the reactor input and the output flows. The typical fermentation temperature of maize is about $35^0$C (Perry and Green, 1999; Ljiljana *et al.*, 2006). The thermal requirements of a fermentation reactor were calculated to be 563 MJ, a value lower than one obtained from literature of 768 MJ (Kim and Dale, 2005a). However the thermal requirements for a distillation column simulated by ASPEN were found to be $1.15 \times 10^4$ MJ which is in good agreement with a literature value of $1.24 \times 10^4$ MJ (Kim and Dale, 2005a).

The fermentation heat requirement is lower than that of distillation by two orders of magnitude, this is due to the fact that it is an exothermic reaction, and thus will only need energy to start the reaction off, as it able to produce its own energy requirements, additionally it would need to be cooled to maintain the required temperature. Coal based electricity and coal-derived steam were assumed to be used to meet these energy needs of the process, a widely practised activity in South Africa, and hence formed an input into the LCI. The energy content of the ethanol product was calculated using a LHV of 25.1 MJ/kg. The resulting energy content of the ethanol product stream was $3.23 \times 10^4$ MJ.

## *Hydrogen production*

### *Mass balance*

The basis for the mass balance for the APR process was taken to be 2.67 tons/hectare of glucose derived from the 3.86 tons/hectare of maize. The same quantity of water of 12.7 $m^3$ of water was assumed, a result of an assumption that was stated in the previous section which is also consistent with literature based data regarding the amount of water required for the process. Calculations were based on a glucose conversion of 98% which is closely related to what was reported in literature of close 100% conversion of glucose into hydrogen (Shabaker *et. al.*, 2003). The amount of hydrogen produced after phase separation is 348 kg, while biogenic carbon dioxide produced is 3.8 tons. The water effluent from the gas liquid separator unit comprises of unreacted water 11.1 $m^3$, with the non-starch containing maize kernels of 1.16 tons. The unconverted glucose of 54 kg forms part of the effluent stream.



### *Energy Balance*

A first order energy balance was carried over the APR reactor. Temperature dependent heat capacities were used for the energy calculations (Coulson and Richardson, 2006). Two reasons can be attributed to the use of temperature dependent heat capacities; a large temperature difference between the reactor inlet and outlet assuming that reactants come into the reactor at 25 $^0$C and exit at about 230 $^0$C, and an involvement of gases whose capacities are more dependent on temperature than that of their liquids counterparts. The thermal requirements for the APR reactor obtained via the energy balance come to 2000 MJ. The thermal requirements of a flash drum were not calculated, rather estimated at 10% that of

the APR reactor, therefore 20 MJ of energy was attributed to it. The reason for this assumption results from the fact that flash drums do not require much energy to achieve phase separation. The energy content of the hydrogen rich product stream based on the LHV of 120.1 MJ/kg of hydrogen is $4.18 \times 10^4$ MJ.

### 3.2.2 LCI output considerations

The material balance provided the input part of the LCI. However, the emissions associated with some of the processes and industrial application options also need to be established. This subsection gives a brief overview of how such data were generated, collected and collated.

The goal of the LCA is to compare the environmental performances of the eight developed scenarios. In order to achieve this, two categories of scenarios were chosen. One broad category investigated the transport-based scenarios and the other was for peak power-based options as stipulated earlier. The input side of these scenarios is well accounted for through material balance, however, the output side is not. Emissions for these scenarios were calculated based on different approaches, hence two types of information sources were used to calculate emissions. The electricity-based electricity options made use of data from Eskom's annual report (Eskom, 2007) and of data sourced from the literature. On the other hand the Greenhouse Gases and Regulated Emissions and Energy use in Transportation (GREET) model (Argonne GREET model, 2006) was mainly used in the emission calculations associated with transport based scenarios. This model allows researchers and analysts to evaluate various vehicles and a fuel combination on a fuel life cycle. The model is also able to model the efficiencies of different vehicles. These aspects will be discussed in more detail in Chapter 4.



## *3.3 Method of LCIA used*

LCIA is aimed at examining the product or process system from an environmental perspective using the impact categories and category indicators connected to the LCI results. It also provides information for the Life Cycle Interpretation phase. According to ISO 14042, it is mandatory that an LCIA should include the following elements:

- Identification of the impact categories, related category indicator and characterisation model, category mid or endpoints and the associated LCA results that the LCA study will address.
- Classification of the LCI results to the impact categories
- Calculation of category indicator results.

**CML 2 Baseline 2000 v2.1**, a method selected for this study, meets all the mandatory requirements of the ISO standard. The method was chosen because it elaborates the problem-oriented (midpoint approach) which was a preferred approach for the study. This method is based on the spreadsheet (version 2.02) as published on the CML website. The CML 2 Baseline method contains several of the impact assessment categories, some of which were chosen in the study in line with the goal and scope of the study. The impact categories with the corresponding category indicators that were chosen for the study as stipulated by the CML 2 Baseline method are summarised below:

#### 3.3.1.1 Climate Change

Climate change can result in adverse effects upon the ecosystems health, human health and material welfare. Climate change is related to emissions of green house gases. The characterisation as developed by the Intergovernmental Panel on Climate Change (IPCC) is chosen for the development of characterisation factors in CML 2. It is these factors that are referred to as Global Warming Potential for a time horizon of 100 years (GWP) in carbon dioxide/kg emissions. The geographical scope of this indicator is at a global scale.

#### 3.3.1.2 Human toxicity

This category involves concerns about the effects of the toxic substances on the human environment. Characterisation factors include Human Toxicity Potentials (HTP) are calculated with USES-LCA, describing fate, exposure and effects of toxic substances for an infinite time horizon. For each toxic substance the HTP's are expressed as 1,4 dichlorobenzene equivalents/kg of emission. The geographic scope of this indicator depends on the fate of a substance and can vary between the local and global scale.

#### 3.3.1.3 Fresh water aquatic-eco toxicity

This category indicator refers to the impact on the fresh water aquatic ecosystems as a result of emissions to air, soil and water. Eco-toxicity Potential (FAETP) are calculated with USES-LCA, describing fate, exposure and the effects of toxic substances. Characterisation factors are described as 1,4 dichlorobenzene equivalents/kg of emission. The indicator applies at global, continental, regional or local scale.

#### 3.3.1.4 Acidification

Acidifying substances cause a wide range of impacts on groundwater, soil, surface water, organisms and buildings. The Acidification Potentials are calculated with an adapted RAINS 10 model, describing the fate and decomposition of the acidifying substances. AP is represented as emissions of $SO_2$ equivalents/kg emissions. Time span is eternity and the geographical scale varies between the local and continental scale.

#### 3.3.1.5 Eutrophication

Eutrophication includes all impacts due to excessive levels of macro-nutrients in the environment caused by emissions of nutrients to air, water and soil. Nutrification Potential (NP) is based on a stoichiometric procedure of Heijungs and Suh (2002) and is expressed as kg $PO_4$ equivalents/kg emissions. Time span is eternity and the geographical scale varies between the local and continental scale.

## *3.4 Comparing different energy products*

Allocation of environmental burdens is seen as a methodological problem in Life Cycle Assessment (LCA) (Azapagic, 1998). By definition it is a process of assigning to each of the functions of a multi function system only those environmental burdens and impacts that are associated with the function. There are two general ways of dealing with the allocation problem: it can be solved by expanding the system boundaries, or by disaggregating the system to understand the real behaviour of the product system sometimes referred to as *casual relationship*.

In this study, the only option of comparing the systems that result in otherwise non-comparable products (power and vehicle travel) is that of expanding the system boundaries by including conventional production of these system functionalities. There are two systems that are under investigation here, the ethanol energy system

and the hydrogen energy systems, analysed on a basis of 8 proposed scenarios. Both systems could produce electricity or transport fuel. When the systems are compared, the conventional (coal or oil-based, systems III and IV) methods of producing electricity and transport fuel need to be added to all the scenarios to compare the scenarios on a similar energy output, see Figure 3.4 below.

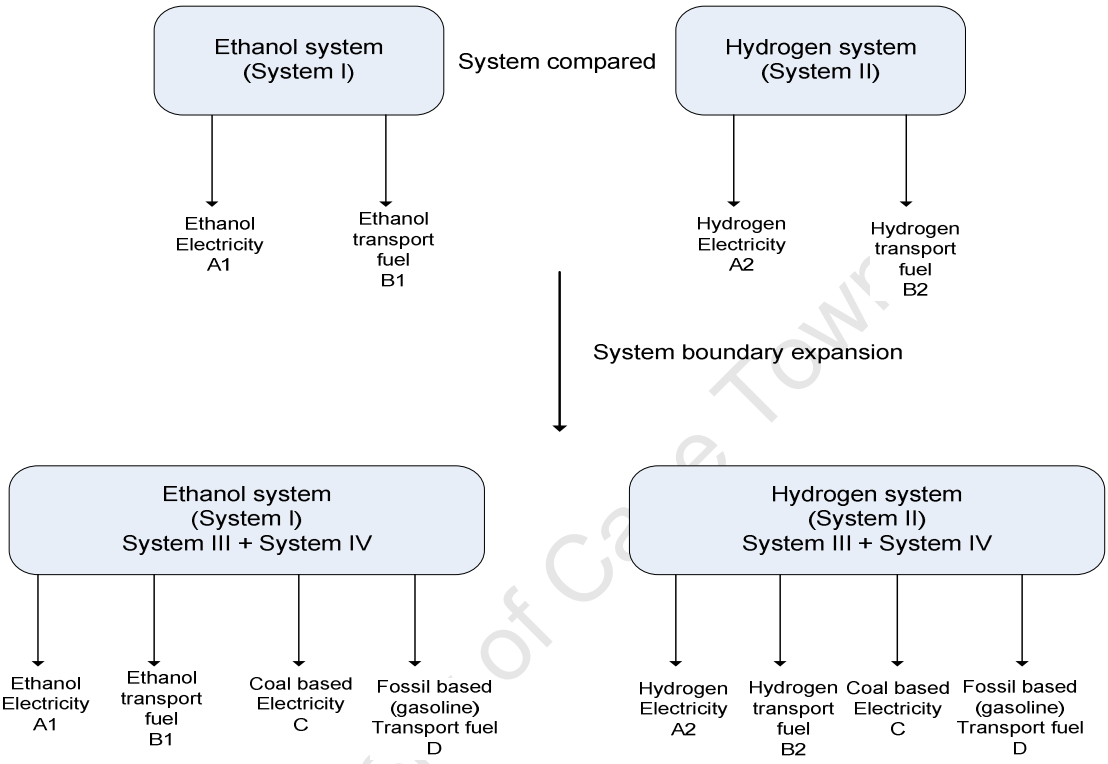


**Figure 3.4: A schematic presentation of a procedure followed for the expansion of system boundaries**

The amount of coal based electricity and/or gasoline that needs to be added to the scenario to result in the same total output in terms of electric energy and vehicle propulsion will differ in the various scenarios due to several factors that will be discussed in more detail in Chapter 4.

## *3.5 Concluding Remarks on the Methodology*

This chapter provided a schematic methodology structured so that the data obtained will be analysed in such a way that the following are met:

i. The aims and objectives of the study are achieved

ii. The hypotheses stated at the start of Chapter 3 are tested.

The subsequent chapters involve the discussion of the data obtained, in the order following the methodology depicted above. Chapter 4 explores environmental performances of the two energy products ethanol and hydrogen via LCA of the 8 proposed scenarios. Chapter 5 discusses one more application of APR produced hydrogen, in a refinery setting.

# 4 Life Cycle Assessment of Electricity and Transport Scenarios

## *4.1 Introduction*

As laid out in the previous chapters, this thesis is centred on a comparative life cycle assessment (LCA) of maize-derived energy products. This chapter firstly defines the goal and scope of this LCA in Section 4.2. Section 4.3 summarises and discusses all the data generated so as to populate the Life Cycle Inventories. A comparative study of the electricity options, and of the transport options, is undertaken in Section 4.4, based on the selected impact categories as stated in Chapter 3. Section 4.5 presents comparative LCA results after system boundary expansion to allow comparison of the 8 industrial applications that have different outputs. The LCA results are interpreted in Section 4.6, and conclusions of the chapter are drawn in Section 4.7.

## *4.2 Goal and Scope Definition*

### 4.2.1 Goal

The primary goal of the study is to analyse the projected environmental performance of the two maize-derived energy products, ethanol and hydrogen. Their performance will be assessed by the impact they have on the environment during production and when used to generate peak power or when used as transport fuel.

The comparative LCA undertaken in this study can be classified as change-oriented or "consequential" following the LCA classification presented in Chapter 2. This type of LCA investigates the likely environmental consequence of decisions that have been proposed for future processes and/or technological application.

The target audience consists of:

i) Researchers involved in bio-energy processes, more specifically, those involved with the life cycle assessment focused on maize-ethanol research.
ii) Policy makers and strategists involved in activities aimed at achieving renewable energy ambitions in South Africa, especially on bio-fuels and the hydrogen economy.

iii) Industry strategists interested in diversifying their product options in the current processes which could complement the existing products, e.g. industries that utilise maize, sugar or other sugar intermediate streams (such as breweries).

## 4.2.2 Scope

### 4.2.2.1 Level of detail

In order to evaluate the 8 generated industrial options, first order input/output mass and energy balances were used to obtain elementary flows for comparison and evaluation of the two energy products from maize. More detailed material balances would need to be carried out over a process flow diagram (PDF), for an advanced LCA analysis.

### 4.2.2.2 System boundaries

The system to be studied is the production of two energy products from maize, ethanol and hydrogen. The ethanol is produced via fermentation and distillation of maize while hydrogen is produced via the 2nd generation bio-energy technology known as the Aqueous Phase Reforming (APR), as introduced in chapter 2.

The production of maize in South Africa averages around 9 million tpa, with a surplus of about 4.5 million tonnes per annum by April 2006 because of overproduction in the previous years (www.grainsa.co.za). This aspect has sometimes resulted in maize prices uncertainty, often times a decrease in the prices. The uncertain and fluctuating maize prices have compelled the leaders in the field to find sustainable alternative uses of maize. One of such options is transforming maize into energy products such as ethanol. The conversion of maize into ethanol is widely practised in the United States of America but is still to be established in South Africa mainly because of its rather modest net energy outputs as discussed in Chapters 1 and 2. Therefore other technologies that are able to exploit the energy content of maize are constantly being researched and developed. The APR is one such technology that is claimed to be able to convert any sugar solution into hydrogen at appropriate conditions.

The two processes for the production of energy products will be briefly presented below. The production process of ethanol will be presented first followed by a brief overview of hydrogen production. The two standard processes used in the commercial ethanol production are the wet-milling and dry-milling methods; the

latter being widely used because of lower costs associated with the erection of infrastructure and relatively higher ethanol yields obtained.

**Dry milling method of producing ethanol**

The first phase in the production process is the grinding of maize kernels into fine meal. Thereafter water and an enzyme called alpha amylase are added to the meal in a process called liquefaction after which the mash is cooked. A second enzyme called gluco-amylase is added to covert starch into sugars in a process called saccharification. Yeast is then added to the mash to ferment the sugars in a process called fermentation, producing ethanol and carbon dioxide. The distillation process follows next, where the ethanol is separated from water and solids. Ethanol is recovered in the distillate and normally has a purity of 95%. The excess water in the ethanol solution is then removed during dehydration which is normally achieved by installing molecular sieves in the system that captures the remaining water and let the vaporised ethanol pass through.

Residual mash and stillage is then transferred from the bottom of the distillation column to the centrifuge where it is normally processed further. The residual mash is normally centrifuged to separate liquid from grain residues. The liquid is then heated to remove water and concentrate the soluble materials. The grain residues can be sold and used immediately to feed cattle within a short space of time, or they can be dried and together with the concentrated syrup and can be sold as livestock feed better known as Dried Distillers Grain with Solubles (DDGS) (Corn Refiners Association, 2005).



**APR for maize**

The second bio-energy product derived from corn is hydrogen. Hydrogen under investigation is produced from oxygenated carbohydrates, in an aqueous phase over an appropriate heterogeneous catalyst at temperatures close to 500K and pressures between 15-60 bar to primarily produce hydrogen and carbon dioxide, (Cortright *et al.*, 2002). This process is called Aqueous Phase Reforming (APR).

The first phase is assumed to be similar to that of ethanol production process where starch is converted into sugars. First the maize kernels are ground into fine meal. Thereafter water and alpha amylase enzyme are added to the meal in the

liquefaction process, after which the mash is cooked. Gluco-amylase is then added to covert starch into sugars in the saccharification process. Thereafter the products of saccharification are fed to the APR reactor where a suitable catalyst is added to the mixture: platinum based catalysts or nickel-tin catalysts are used for the selectivity of the reaction towards hydrogen. The APR products are separated in a phase separator where the hydrogen rich gas stream is separated from the liquid and solid stream. The next stage is that of hydrogen purification where hydrogen is separated from the other gas products such as carbon dioxide and some of alkanes that might have been produced in small quantities from competing reactions.

Both the processes for ethanol and hydrogen production are similar up to the saccharification stage, therefore all the processes prior to this stage are omitted in the LCA as the environmental burdens incurred from harvesting to processing of maize into a sugar solution are identical. The environmental performances of the energy products will be compared on a basis of their application either as transport fuel or electricity generated. Therefore, the LCA analysis system boundaries will begin at either fermentation or APR and end with the combustion of the energy products, either as transport fuel in motor vehicles, or in a peak-power producing electricity plant. The diagram below depicts the system boundary chosen for this study, in line with the objectives and goal; the dotted line illustrates the boundary for the life cycle study.

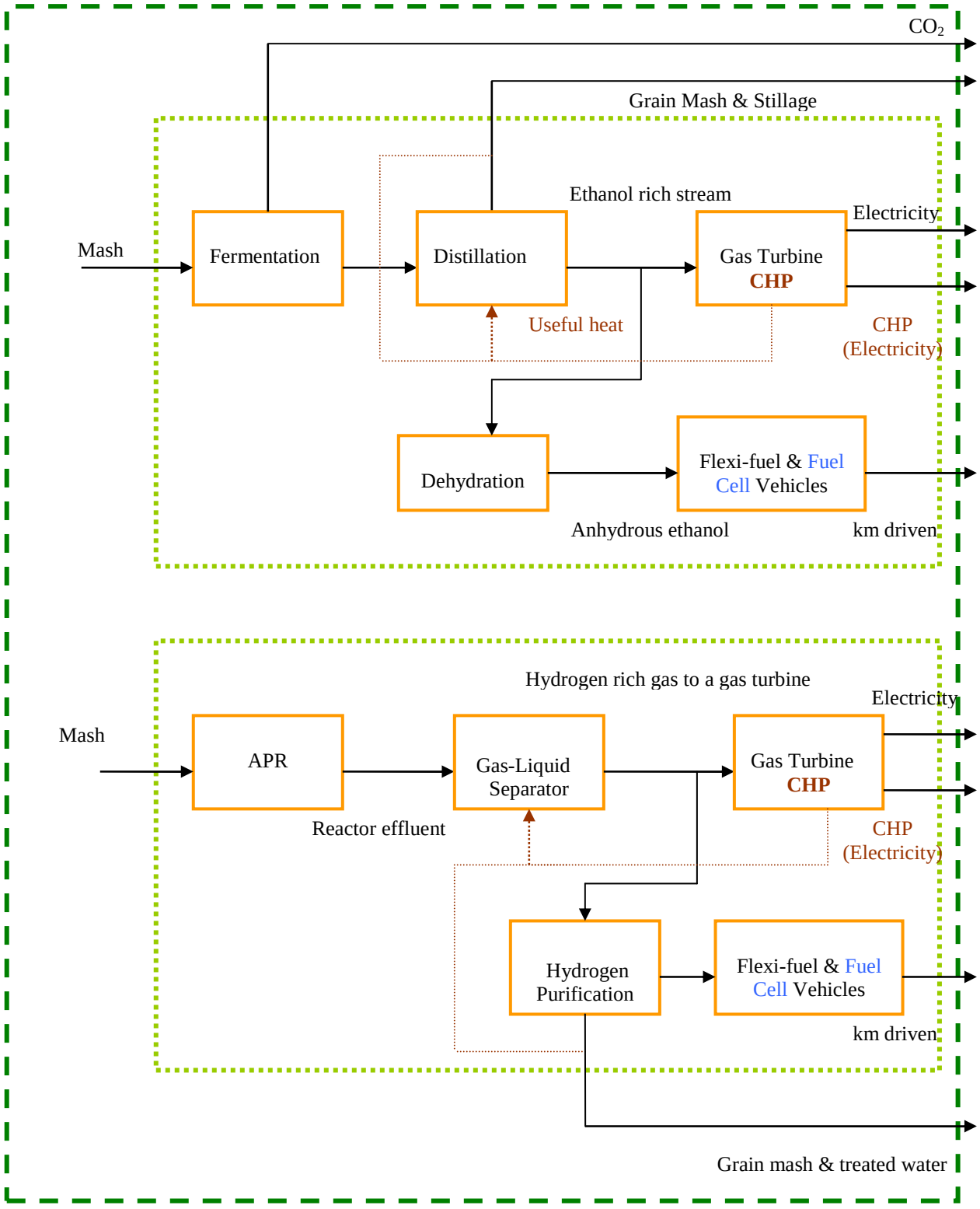


**Figure 4.1: System boundary for the life cycle study**

#### 4.2.2.3 Functional Unit

The functional unit for the systems under investigation is the service rendered by maize produced energy products as either peak power electricity or transport fuel that could be derived from maize harvested from 1 hectare of land in South Africa under current farming. The yield that results from the land is 3.86 tons of maize which is the feedstock to either of the processes under investigation. The functional unit is a basis for data tabulation and calculations and hence all data is reported on this basis. The bioenergy systems are measured by the amount of ethanol and hydrogen produced from the reference flow. The electricity production scenarios are measured by the amount of electricity produced in MJ. The transport fuel options are measured by vehicle mileage when run on ethanol and hydrogen in a normal and in fuel cell vehicles.

#### 4.2.2.4 Data categories and quality

The system inputs have been modelled as elemental where possible, while the data used is partly based on industrial data, literature and assumptions. Average data values connected with maize production, ethanol production process, and the APR processes have been used in the calculations and analysis. The data obtained from different sources was deemed sufficient to compile data that will meet both the objectives and the goal and the scope of the study.

The data pertaining to the maize yields is widely available and well documented by major players in the farming industry. The emissions from all the systems have been made inclusive where possible, and the process blocks depicted in Figure 4.1 encompass emissions to air, water and soil. The data for processing was sourced from similar literature studies. Most of the options under comparison are reliant on the use of fossil coal to meet the process thermal needs, which is known for the range of pollutants it emits. The main gases of concern include carbon dioxide, nitrogen oxides, sulphur dioxide and particulates, while COD and BOD will determine the impact on the water. Suitable impact categories were selected based on the type of emissions given off in systems under analysis; these were supported by the ones selected in similar studies on LCA of bioenergy systems as discussed in Chapter 2. The following impact categories were chosen as stated in Chapter 3: Global Warming Potential, Acidification Potential, Eutrophication, Human Toxicity and Fresh Water Eco-toxicity.

This study is a pre-feasibility environmental analysis exercise; therefore the value placed on the quality of the data was not as strict it would be for a very detailed environmental analysis, which would be carried out subsequently. It should also be noted that the data used for the hydrogen production process will not have the same accuracy as that of ethanol production process as APR process is still undergoing research and development and has not been operated on a large scale. However, data quality in this study, like in many LCA studies is still considered very important for the presentation of accurate and sound results. Therefore the best possible data was sourced and used for the calculations. The technological data was sourced for current (ethanol production) and near future (APR) due to the comparative nature of the study that required the systems to be compared on a similar level. The individual data categories were evaluated with the aid of the pedigree matrix (Weidema and Wesnaes, 1996). The following data quality requirements will be addressed; i) time related coverage, ii) geographical coverage, iii) precision, completeness and representativeness of data, iv) consistency and reproducibility of the methods throughout the LCA, v) sources of data and their representativeness, vi) uncertainty of the information.



**Table 4.1: Data quality indicators**

| **Bio-ethanol system** | **Score** | | | | |
|---|---|---|---|---|---|
| Process | Reliability | Completeness | Temporal | Geographical | Technolgical |
| | | | | | |
| Maize production | 2 | 2 | 2 | 1 | 2 |
| Fermentation | 3 | 3 | 3 | 3 | 3 |
| Distillery | 3 | 3 | 3 | 3 | 3 |
| Electicity production | 3 | 3 | 3 | 4 | 3 |
| Transport emissions | 2 | 3 | 3 | 4 | 3 |
| Coal electricity | 2 | 3 | 2 | 1 | 3 |
| | | | | | |
| **Bio-hydrogen system** | **Score** | | | | |
| Process | Reliability | Completeness | Temporal | Geographical | Technolgical |
| | | | | | |
| Maize production | 2 | 2 | 2 | 1 | 2 |
| APR | 4 | 4 | 4 | 4 | 3 |
| Electicity production | 2 | 2 | 3 | 3 | 3 |
| Transport emissions | 3 | 3 | 3 | 4 | 3 |
| Coal electricity | 1 | 3 | 2 | 1 | 3 |

The matrix highlights the areas of concern, the higher the number the less reliable the data is. Amongst the 5 indicators presented above, completeness and reliability scores are regarded the most important for this study, while the others should be treated relative to the process at hand.

#### 4.2.2.5 System descriptions

There are 8 options under consideration in this comparative LCA. Firstly, there are the two electricity generation options, one from each of the maize derived energy products, referred to as ethanol electricity (EE) and hydrogen electricity (HE). There are two more electricity options resulting from heat integration into the base electricity generation options, which are termed ethanol and hydrogen electricity with heat integration (EE-HI and HE-HI). Four transport based options are also investigated; for ethanol the two types of vehicles were chosen and can be abbreviated as E-FFV and E-FCV for ethanol flexi fuel and fuel cell vehicles, while for hydrogen an internal combustion engine and fuel cell vehicles were chosen ($H_2$-ICEV and $H_2$ FCV) The processes systems under investigation are presented in Figures 4.2 to 4.5 below.

**Electricity generation options**

The primary product of the options presented below is electricity. The amount of electricity generated in both cases depends on assumed gas turbines efficiencies which could be achievable according to the literature. Ethanol and hydrogen rich streams are not purified further in the electricity options because gas turbines are able to handle a mixture of gases/liquid products as feed. In both the production of ethanol via fermentation and distillation and that of hydrogen from the APR, carbon dioxide is given off as a by-product that can be purified and possibly sold to suitable industries.

The significant difference between the basic peak power options and the ones with heat integration is that the latter also harnesses the heat of combustion gases through a combined heat and power (CHP) configuration. CHP technology is an energy conversion process whereby electricity and useful heat are produced simultaneously in one process using heat exchangers to recover process heat (Cohen, 2006). There are two ways in which heat can be integrated in the electricity generation options. First, the exhaust gases from the gas turbine are fed through a

heat recovering unit in a CHP configuration. Secondly, the anaerobic digestion of stillage (after recovery of DDGS, and similarly of the grain mash in APR) produces biogas which can either be converted to heat or power or both in a CHP process; for the purpose of this study it was assumed that energy product derived from biogas was useful heat only. All heat produced or recovered through process integration reduces the amount of coal-based heat required by the processes as presented in Figures 4.2 and 4.3. Coal-based electricity as per practice in South Africa is used to drive the processes.

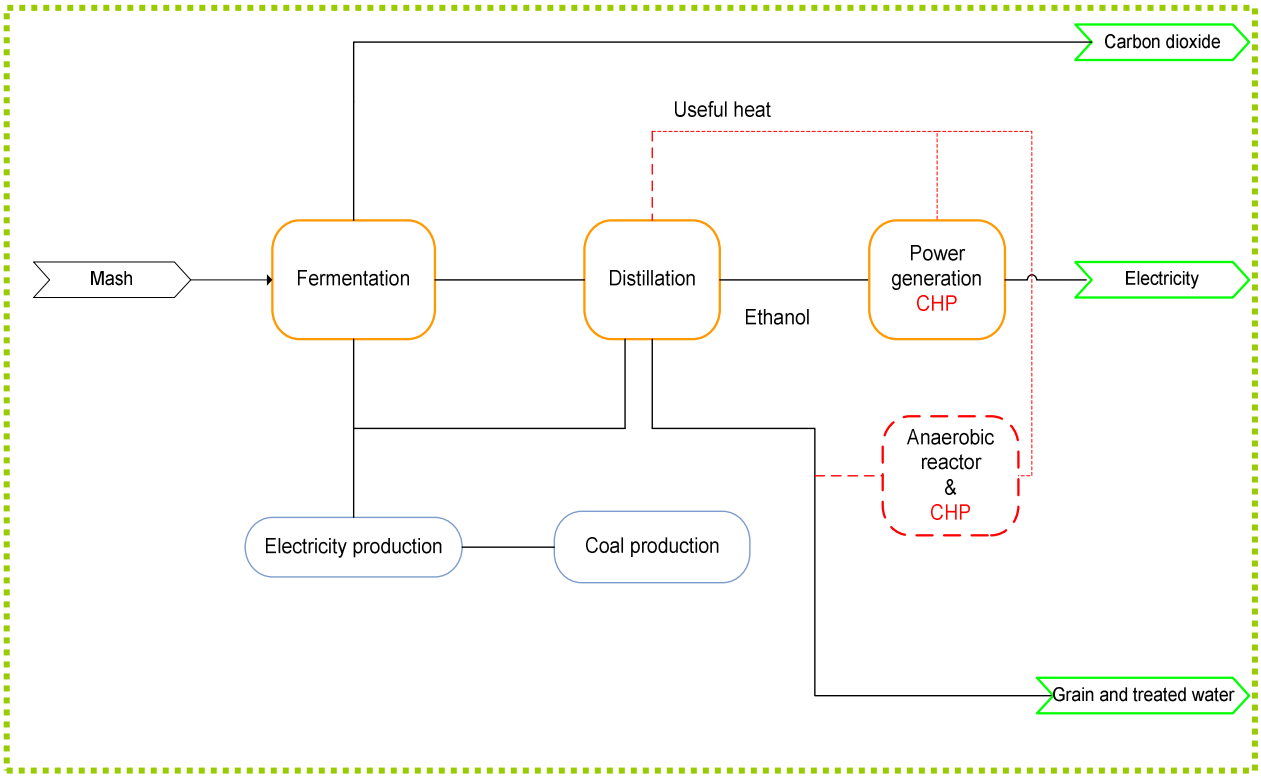


**Figure 4.2: Life cycle diagram illustrating the ethanol electricity options**

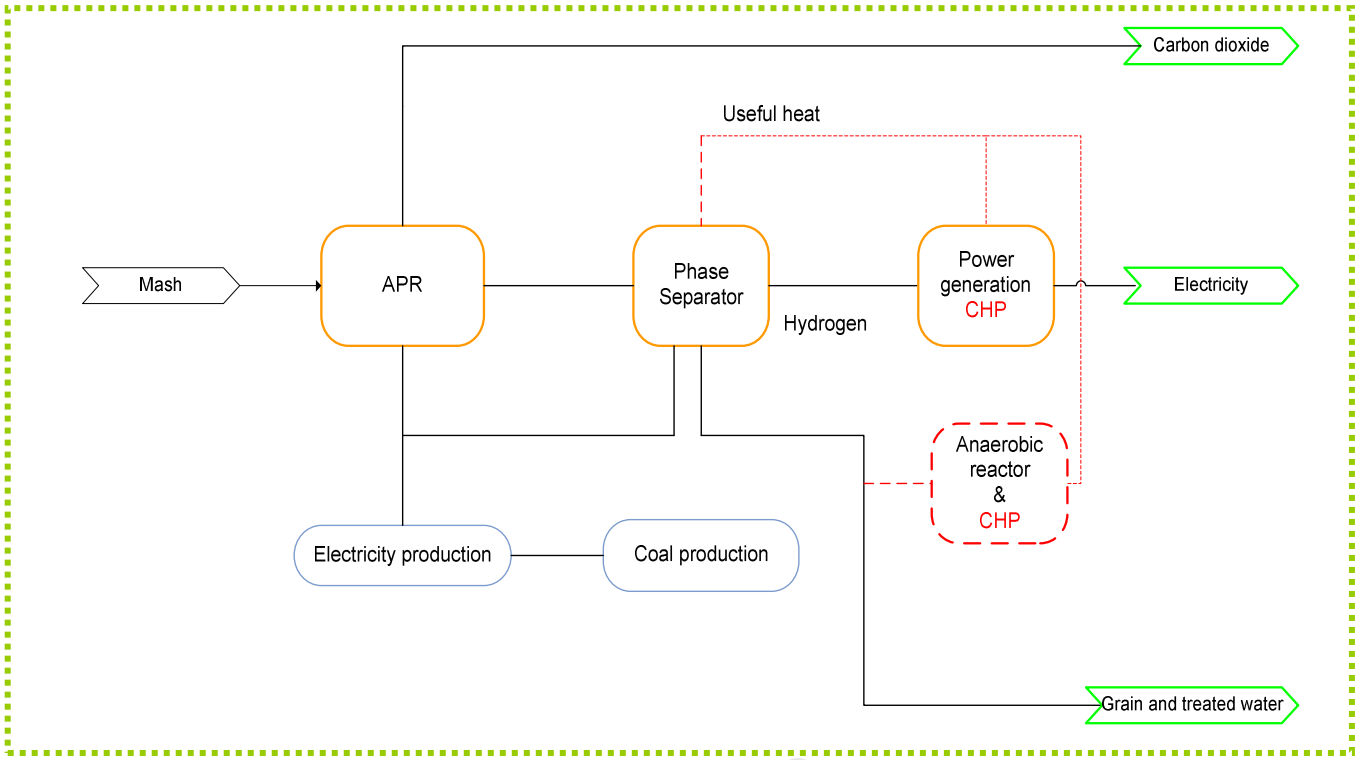


**Figure 4.3: Life cycle diagram representing the hydrogen electricity options**

## Transport options

The primary product of the transport fuel options is the number of kilometres that can be driven when using ethanol or hydrogen fuels. Ethanol used as transport fuel needs to be at least 99.5% pure, while hydrogen rich gas also needs to be purified to meet the standard that can be used as vehicle fuel. Two types of vehicles were chosen for the two transport fuels. The flexi-fuel and fuel cell vehicles were selected for ethanol fuel, while an internal combustion engine (ICE) and fuel cell vehicles were selected for hydrogen fuel. The efficiencies of these four vehicle types, and hence the amount of kilometres achievable based on the functional unit were based on the GREET model latest modification of 2007 (Argonne Laboratory, 2006).

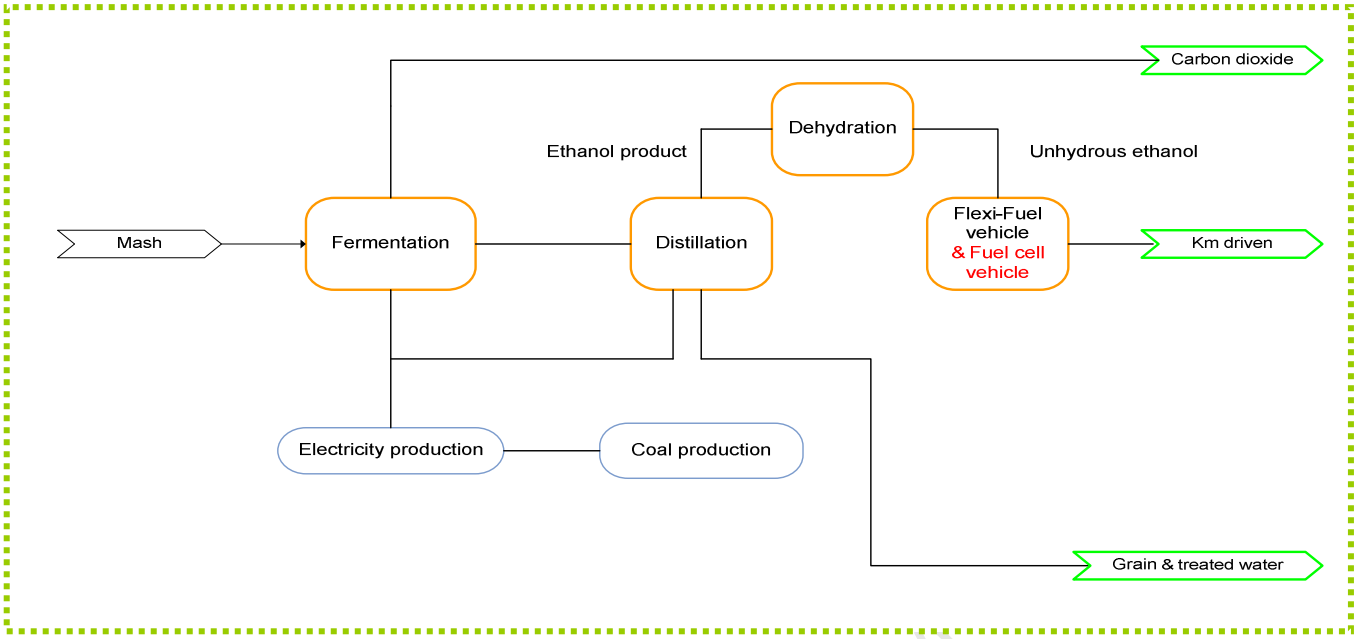


**Figure 4.4: Life cycle diagram for the ethanol transport options**

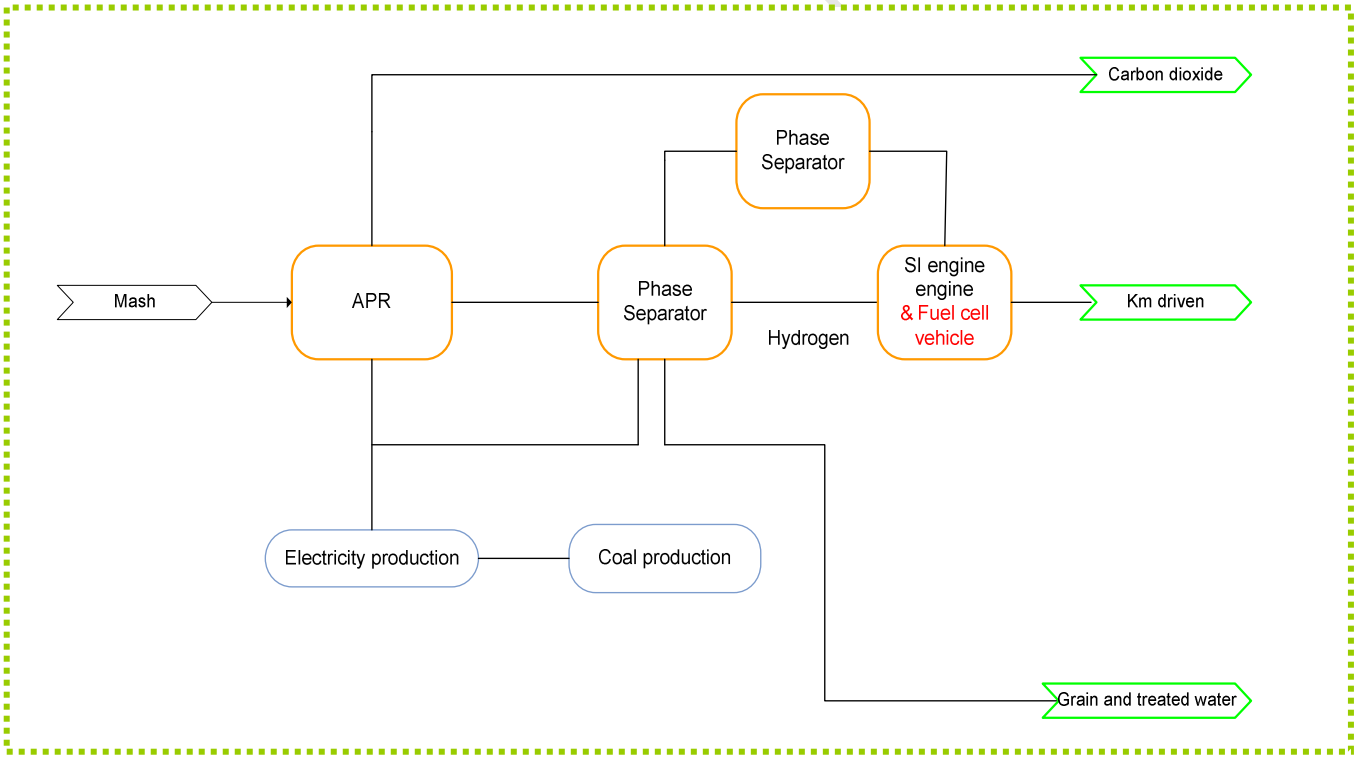


**Figure 4.5: Life cycle diagram for the hydrogen transport scenarios**

## *4.3 Inventory Analysis*

### 4.3.1 Introduction

Proceeding from the goal definition and the scope of the LCA study presented in Section 4.2, this section analyses the Life Cycle Inventory Data (LCI) compiled according to methods presented in Chapter 3. The data used was collected from numerous sources. Studies of the same nature were consulted for input of various processes because of lack of industrial data which is primarily due to the nature of technologies under investigation in the South African context, although not entirely accurate, the data used provides a good estimate for further modelling of the systems.

The assessment and inventory was completed using process knowledge and various literature sources to support it. Block flow analysis was applied to major unit processes. A first order mass and energy balance was made over the blocks, where data was not available assumptions were made to compete the investigation. These assumptions were documented in Chapter 3 and in detailed calculations presented in Appendix B.

All data collected were related to maize that could be derived from 1 hectare of land in South Africa under current farming, which was estimated at 3.86 tons/hectare (www.grainsa.co.za). All the data pertaining to energy consumption and emissions were based on this reference flow. It was considered useful thereafter to group data compilation according to the two production technologies for the two energy products, ethanol and hydrogen, and for the different use options, electricity generation and transport. Subsections 4.3.2 and 4.3.3 discuss briefly how the summarised data were compiled.

## 4.3.2 Ethanol production process

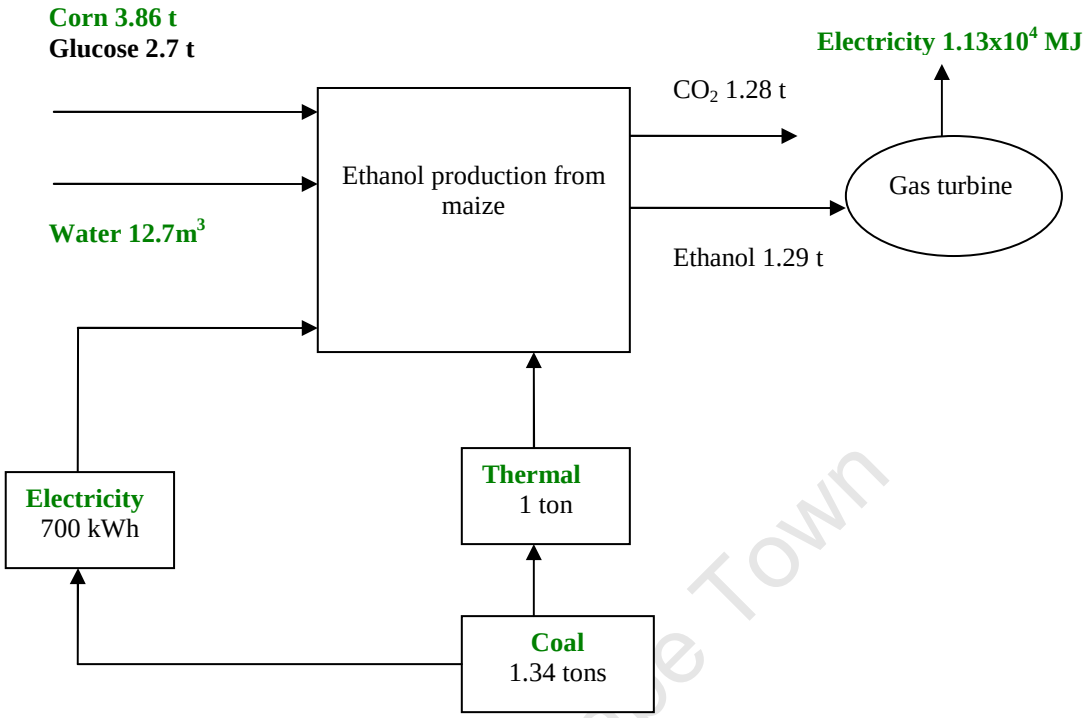


**Figure 4.6: Summary flows for the ethanol electricity option**



### *Fermentation*

Figure 4.6 summarises major flows in the ethanol production process based on the methodology and assumptions outlined in Chapter 3. The amount of sugar fed into the fermentation process was based on the reference flow of 3.86 tons/hectare of maize yields which translated into 2.7 tons of glucose can be derived . The amount of water used was 12.6 $m^3$. The energy required for the process was obtained through energy balance calculation and supported by literature at 770 MJ.). Coal will be used to meet the thermal requirements while coal based electricity will be employed as typical of the South African industrial practice.

### *Distillation*

The amount of ethanol produced from the distillation unit is 1.29 ton. The energy input calculated for distillation is 1.32 x $10^4$ MJ, which was in agreement with literature. lThe electricity requirements amount to 700 kWh, while the total amount of coal use for process heating and electricity generation amounts to 1.34 tons. The product that comes from the bottoms of the distillation column comprises of water

and spent grain, which are 11.6 $m^3$ and 1.64 tons respectively. The electricity option with heat integration was calculated to use 0.1 ton of coal, however has similar stillage composition.

### 4.3.3 Hydrogen production process

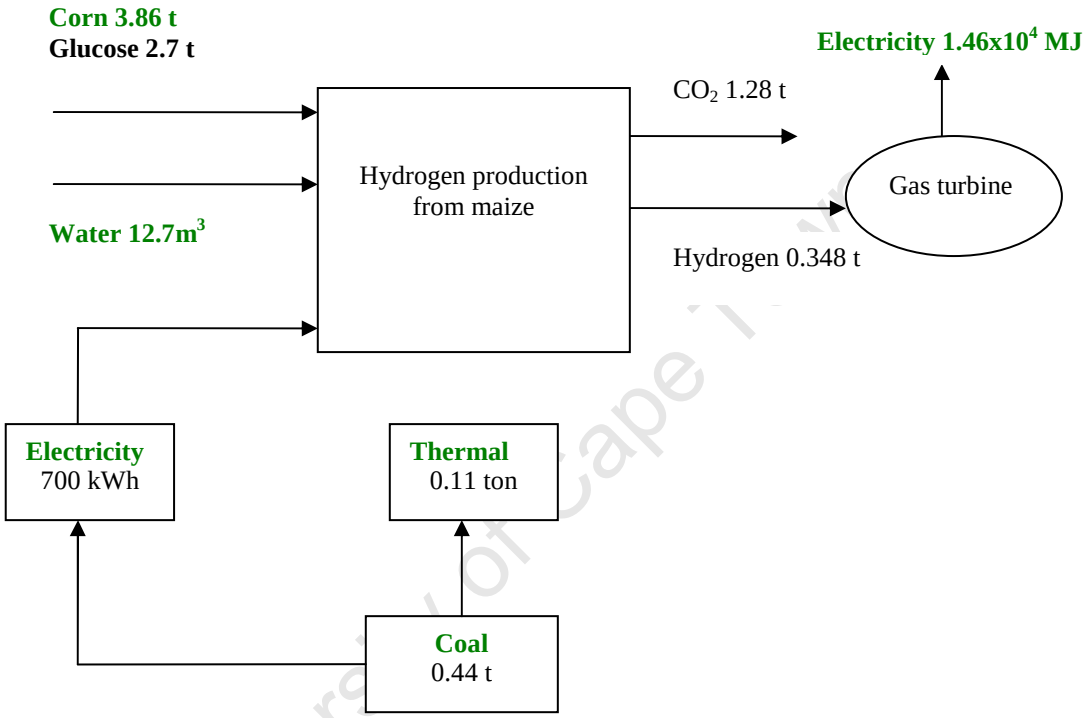


**Figure 4.7: Summary flows for the APR process**

***Aqueous phase reforming***

Figure 4.7 summarises the material flows of the hydrogen production process as outlined in the methodology in Chapter 3. The same amount of sugar, 2.7 tons of glucose will be used according to the reference flow. Since a similar concentration of sugar in water was assumed to that required for fermentation, a similar quantity of water was used for the APR process at 12.6 $m^3$. There were no literature data to support the energy requirement value that was obtained from energy balance. Energy requirements obtained from the first order energy balance was 2500 MJ which translates to 0.11 tons of coal. The electricity requirements of the process were assumed to be similar to those of an ethanol flow sheet (700 kWh), since no information is available in the literature. This will include all the electricity requirements for both the APR reactor and the phase separator. The liquid and solid

that are recovered in the solid and liquid phase amount to 11.1 $m^3$ of water and 1.16 tons of spent grain.

### 4.3.4 Electricity Options data summary and data compilation

Table 4.3 presents a summary of life cycle inventory for the electricity options:

**Table 4.2 : Inventory summary for the electricity options**

| Flow | Units | EE | HE | EE-HI | HE-HI |
|---|---|---|---|---|---|
| *Inputs (products)* | | | | | |
| Corn | t | 3.86 | 3.86 | 3.86 | 3.86 |
| Glucose | t | 2.67 | 2.67 | 2.67 | 2.67 |
| Coal (process heating) | t | 1.01 | 0.11 | 0.02 | -1.4 |
| Coal (electricity) | kWh | 700 | 700 | 700 | 700 |
| Water tot. | litre | 12685 | 12685 | 12685 | 12685 |
| (Hydrogen) | kg | - | 348 | - | 348 |
| (Ethanol) | kg | 1286 | - | 1286 | - |
| (Electricity) | MJ | 1.13E+04 | 1.46E+04 | 1.13E+04 | 1.46E+04 |
| (Land Use) | $m^2$ | 1.00E+04 | 1.00E+04 | 1.00E+04 | 1.00E+04 |
| | $m^2$/MJ | 8.85E-01 | 6.84E-01 | 8.85E-01 | 6.84E-01 |
| *Outputs* | | | | | |
| (AIR) Carbon dioxide, (fossil) | t | 2.10 | 0.73 | 0.56 | 0.50 |
| (AIR) Carbon dioxide, (biogenic) | t | 3.92 | 3.90 | 3.92 | 3.90 |
| (AIR) Carbon monoxide | kg | 1.99 | 0.273 | 1.88E-01 | 1.15E-01 |
| (AIR) Methane (fossil) | kg | 6.8 | 0.4 | 2.38 | 2.21 |
| (AIR) Nitrogen oxides | kg | 8.3 | 6.0 | 4.44 | 5.36 |
| (AIR) Particulates emissions | kg | 0.14 | - | 0.20 | - |
| (AIR)Sulphur dioxide | kg | 13.56 | 5.54 | 0.00 | - |
| (WATER) BOD (Biological Oxygen Demand) | t | 0.67 | 0.26 | 0.60 | 0.26 |
| (WATER) COD (chemical oxygen demand) | t | 0.83 | 0.36 | 0.82 | 0.36 |
| (WATER) Nitrate | kg | 2.61E-03 | 8.00E-04 | 5.69E-04 | 4.84E-04 |
| (WATER) Spent corn | kg | 1.16E+03 | 1.16E+03 | 1.16E+03 | 1.16E+03 |



Major and intermediate streams for these options were discussed in previous sections. Data for the associated emissions for the electricity options were based on literature on gas turbines (Strachan and Farrel, 2006).

## 4.3.5 Transport Scenarios data compilation

**Table 4.3 : Inventory summary for the transport options**

| Flow | Units | E-FFV | E-FCV | $H_2$-ICEV | $H_2$-FCV |
|---|---|---|---|---|---|
| *Inputs* | | | | | |
| Corn | t | 3.86 | 3.86 | 3.86 | 3.86 |
| Glucose | t | 2.67 | 2.67 | 2.67 | 2.67 |
| Coal (process heating) | t | 1.01 | 1.01 | 0.11 | 0.11 |
| Coal (electricity) | kWh | 700 | 700 | 700 | 700 |
| Water tot. | litre | 12685 | 12685 | 12685 | 12685 |
| Hydrogen | kg | - | - | 348 | 348 |
| Ethanol | kg | 1286 | 1286 | - | - |
| Distance travelled | km | 1.07E+04 | 1.59E+04 | 1.66E+04 | 3.22E+04 |
| Land Use | $m^2$ | 1.00E+04 | 1.00E+04 | 1.00E+04 | 1.00E+04 |
| | $m^2$/km | 0.93 | 0.63 | 0.60 | 0.31 |
| *Outputs* | | | | | |
| (AIR) Carbon dioxide, (fossil) | t | 2.20 | 2.19 | 0.74 | 0.74 |
| (AIR) Carbon dioxide, (biogenic) | t | 3.98 | 3.98 | 3.90 | 3.89 |
| (AIR) Carbon monoxide (biogenic) | t | 0.03 | 0.02 | 0.01 | 0.00 |
| (AIR) Carbon monoxide (fossil) | kg | 2.04 | 2.02 | 0.39 | 0.39 |
| (AIR) Methane (fossil) | kg | 7.08 | 7.05 | 2.91 | 2.90 |
| (AIR) Nitrogen oxides | kg | 5.73 | 6.90 | 5.83 | 4.80 |
| (AIR) Particulates emissions | t | 3.54E-01 | 4.73E-01 | 0.49 | 0.80 |
| (AIR)Sulphur dioxide | kg | 1.38E+01 | 5.56E+00 | 1.44E+01 | 5.73E+00 |
| (WATER) BOD (Biological Oxygen Demand) | t | 0.62 | 0.21 | 0.27 | 0.27 |
| (WATER) COD (chemical oxygen demand) | t | 0.86 | 0.47 | 0.37 | 0.37 |
| (WATER) Nitrate | kg | 0.02 | 0.44 | 0.00 | 3.19E-04 |
| (WATER) Spent corn | kg | 1.16E+03 | 1.16E+03 | 1.16E+03 | 1.16E+03 |



A summary of the major flows for the transport-fuel scenarios are presented in Table 4.3 above. As discussed in chapter 3, the vehicle emission data for the transport options were compiled with the aid of GREET model which is a tool that quantifies the energy use and emissions of present and advanced technologies and new transportation fuels. This model was used for all the four vehicle options chosen for analysis.

## *4.4 Comparison of ethanol and hydrogen options*

An LCIA was used within the LCA to compare the ethanol and hydrogen production options within the electricity generation scenario on the one hand, and within the transport options on the other, in order to obtain insights into environmental issues associated with the use of resources and emissions as gathered and compiled in the LCI. As mentioned in chapter 3, mid-point indicators were employed for the impact categories of Global Warming, Human Toxicity, Acidification, Fresh Aquatic Eco-toxicity and Eutrophication. The LCA software package SimaPro version 7.0 was used to undertake the LCA while ***CML 2 baseline 2000 v2.1 (***which elaborates the problem-oriented (mid-point) approach) was the selected method for the analysis. Although land use cannot be classified as an impact category per se, it was used here to obtain an indication of the efficiency of land use for producing the maize energy products ethanol and hydrogen.

### 4.4.1 Ethanol vs. hydrogen production

Based on the inventory results shown in Tables 4.2 and 4.3, it is not surprising that the four hydrogen options outperform the four ethanol options in all impact categories considered, as shown in Figures 4.8 and 4.9 below. The following sections will carry out a comparative exercise to identify the cause of the dominance displayed by the hydrogen options over the ethanol ones.

### 4.4.2 Incorporation of heat integration into the electricity options

Heat integration decreases the amount of coal required to meet process heating in the production of ethanol and hydrogen. The ethanol thermal requirements are reduced tremendously while the hydrogen ones were replaced completely, in fact, excess process heat could be generated, this could either be exported to other industries or diverted to the production of electricity instead of just heat (especially from the one produced from biogas).

The impact categories that are directly linked to the intensive use of coal, such as global warming, acidification, human toxicity and fresh water aquatic eco-toxicity are strongly reduced for both the products after heat integration as indicated in Figure 4.8. The ethanol electricity production option with heat integration had these impacts reduced by over 90% compared to just ethanol electricity option. The impacts

associated with process heating for hydrogen production were eliminated, the contribution is due to coal-based electricity. This trend is not evident in eutrophication and land use as their indicators are not dependent on coal use.

### 4.4.3 Efficiency of land use

Although it was mentioned earlier that land use is not one of the impact categories that are presented by the method chosen, CML 2000, it was evaluated to investigate the efficiency of using land for the two energy products. This is a direct result of the energy yields of the processes, deduced for maize harvested from 1 hectare of land. It was found difficult to compare the land use efficiency for transport and electricity options; instead the efficiency was explored for products within an energy application, i.e. for electricity and transport separately. The results show that use of land for hydrogen production is more efficient than that of ethanol production in either of the application, electricity and transport. This result is in agreement with the modest energy yield in ethanol compared to that in hydrogen from a similar reference flow and as discussed in Chapters 1 and 2.

### 4.4.4 Comparing the results within impact categories for electricity options

This section discusses the different impact assessment categories that were used to assess the inventory results. The inventory results of the four electricity options will be dealt with here. Impact categories that are discussed are mentioned earlier, and also presented in Figure 4.8. The subsequent subsections will discuss the individual impact categories and their contributing sub-processes. The following section gives rigorous account and analysis of the impact categories for individual options. The reader may choose to skip this section and proceed to Section 4.5.6 for an analysis of the options after system boundary expansion.

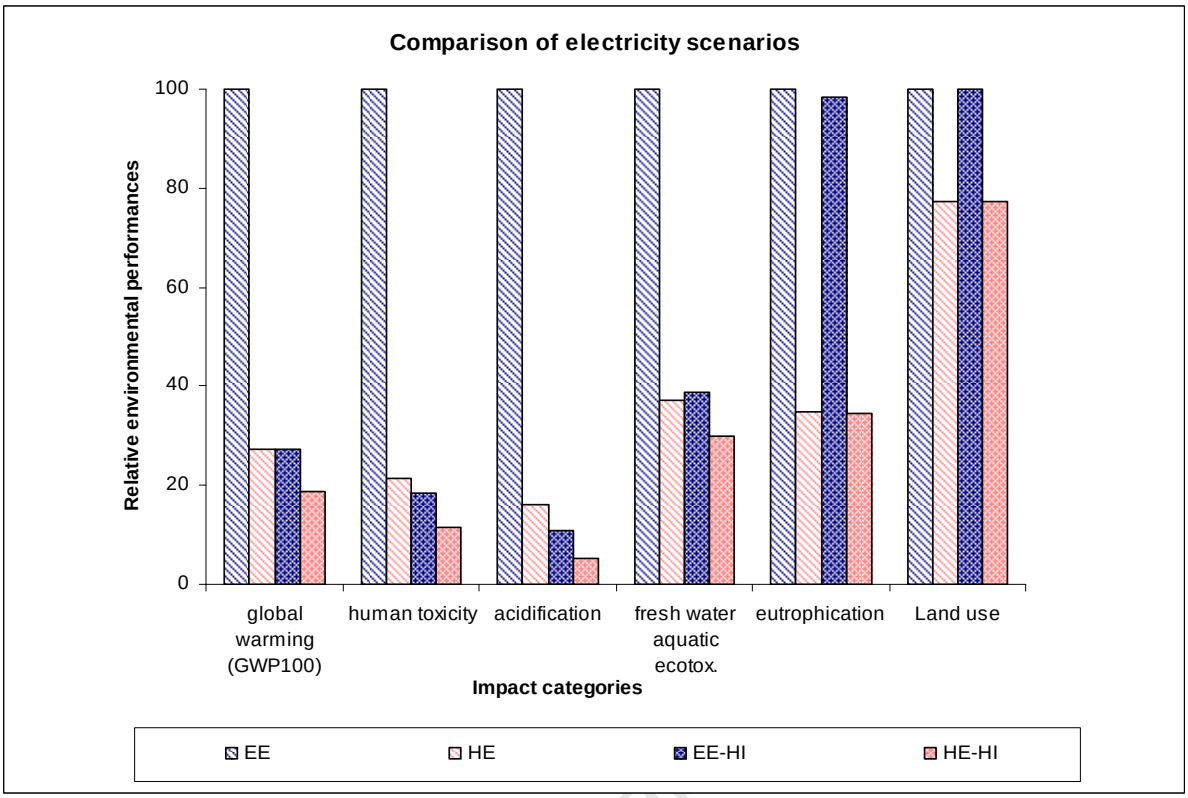


**Figure 4.8 : Comparison of environmental performances for electricity options per MJ of electricity generated**

### 4.4.4.1 Global warming potential

This impact category is related to green house gases emissions, as explained in section 3.3. It can be observed from Figure 4.8 and Table 4.3 that the EE option displays the highest global warming impact contribution of 0.20 kg $CO_2$ equiv. per MJ of electricity generated, this was expected as the production of ethanol is the most coal intensive in comparison with all the other options. Coal combustion results in carbon dioxide emissions, whilst methane is released during coal mining. The amount of coal needed to meet thermal requirements for the production of ethanol is 1 ton while that of hydrogen was worked out to be 0.11 ton from fist order material balance; therefore the resulting green house emissions are higher by a factor of 10 for ethanol production. Similar electricity requirements for ethanol production of 700 kWh coal based electricity were used for APR due to unavailability of data, hence total amount of green house associated with the two production systems should be the same, however will be lower per MJ of electricity generated for the APR due to better energy yields. The resulting Global Warming Potential for the EE is higher than that of HE by about 70%. EE-HI and HE-HI show a much more improved global warming potential, a result also of reduced usage of coal, for ethanol production the

amount of coal requirements was reduced from 1 ton to 0.02 ton and was eliminated altogether for hydrogen production from 0.11 tons with a potential heat export equivalent to burning 1.4 tons of coal. This implies that more process heat is produced for the hydrogen process than is needed by the process. However the global warming impact due to electricity use remains the same after heat integration as only coal for process heat is replaced, as presented in Table 4.4.

The global warming potential can be summed up as follows: the hydrogen electricity options present better environmental performance than ethanol electricity options, for both with and without heat integration. Heat integration reduces the global warming potential tremendously for both the fuels, even more so for EE. Table 4.4 quantifies the contribution per process, and shows that heat from coal and coal based electricity are the highest global warming potential contributors, and EE has the highest contribution, while HE-HI has the lowest due to less intensive coal use and better process efficiencies.

**Table 4.4: Major process contribution to global warming potential for the electricity options in kg $CO_2$ equivalence per MJ of electricity generated**

| Process | EE | HE | EE-HI | HE-HI |
|---|---|---|---|---|
| **Total of all processes** | **2.00E-01** | **5.47E-02** | **5.44E-02** | **3.73E-02** |
| | | | | |
| Heat, from hard coal | 1.51E-01 | 1.74E-02 | 6.01E-03 | 3.43E-03 |
| Electricity coal, ZA | 4.26E-02 | 3.29E-02 | 4.26E-02 | 3.29E-02 |
| Hard coal, at mine | 4.44E-03 | 3.43E-03 | 4.44E-03 | 1.89E-05 |
| Hardwood, allocation | 4.35E-04 | 3.35E-04 | 4.35E-04 | 2.70E-04 |



#### 4.4.4.2 Human toxicity

The complexity in the evaluation of this impact category (measured in 1,4-DB equivalents) results from the contribution of a number of substances which is not as straightforward as the evaluation of global warming potential, these range from benzene, via priority air pollutants such as sulphur dioxide and nitrogen dioxide, to some metal substances such as chromium and nickel. However, the trend for this impact category still follows that of global warming potential.

Table 4.5 shows that the highest contribution to potential human toxicity emanate from the use of coal for process heating, with that of coal based electricity an order of magnitude lower. If EE is taken as an example, it can be observed that the total contribution of all processes to human toxicity amounts to 5.49 x $10^{-2}$ kg 1,4-DB

equiv. per MJ of electricity generated with coal usage contributing over 80% at 4.67 $x10^{-2}$ kg 1,4-DB equiv. In all the options except the HE-HI where only coal based electricity was required for hydrogen production this trend was evident, where the electricity emissions contribute over 80%. Because of the intensive use of fossil fuel and the lower process efficiency in the ethanol production, the human toxicity is higher compared to the more efficient one of the APR. Heat integration reduces the amount of human toxicity impact; less coal use infers relatively less toxic materials to humans are released.

**Table 4.5 : Major process contributions to human toxicity for the electricity options in kg 1,4-DB equivalence per MJ of electricity generated**

| Process | EE | HE | EE-HI | HE-HI |
|---|---|---|---|---|
| **Total of all processes** | **5.49E-02** | **1.18E-02** | **1.00E-02** | **6.39E-03** |
| | | | | |
| Heat, from hard coal | 4.67E-02 | 5.37E-03 | 1.85E-03 | 6.63E-05 |
| Electricity coal, ZA | 7.39E-03 | 5.70E-03 | 7.39E-03 | 5.70E-03 |
| EE emissions | 2.70E-04 | - | - | - |
| HE emissions | - | 2.76E-04 | - | - |
| EE-HI emissions | - | - | 2.45E-04 | - |
| HE-HI emissions | - | - | - | 2.76E-04 |



### 4.4.4.3 Fresh water aquatic eco-toxicity

Figure 4.8 presents the impact category for fresh water aquatic-eco-toxicity, which follows a similar trend to the two impact categories discussed above, Global Warming Potential and Human Toxicity Potential. This can be explained with the aid of Table 4.6 which shows the contributing processes to the category.

Coal use is still dominant in this impact category as in the other two. Taking the EE option as an example once more, it is shown that for a total processes' emissions of 6.96 x $10^{-3}$ kg 1,4-DB equiv., process heat coal's contribution is 6.10 $x10^{-3}$, which amounts to more than 90% of all the processes. The next highest contribution comes from the use of coal based electricity. Therefore the less the coal utilised in a process the less the Fresh Water Aquatic Eco-toxicity impact. HE-HI's contribution to this impact category is primarily due to coal based electricity; however it still exhibits the best performance under this category compared to the other options. Again the usage of coal as supported in Chapters 1 and 2 does have a negative impact on the eco-system. Although one would have thought that water discharged from ethanol and hydrogen production would make a contribution to fresh water aquatic eco-

toxicity, this was not the case because the COD of the effluent streams was used instead of the individual organic components of the effluent, the LCA method employed was not able to analyse them. One observation that has surfaced in all the impact categories is that their performances are dominated by the production phase of bio fuels only negligible contributions are due to their end use, in this case electricity generation.

**Table 4.6: Major process contribution to fresh water aquatic eco-toxicity for the electricity options in kg 1,4-DB equivalence per MJ of electricity generated**

| Process | EE | HE | EE-HI | HE-HI |
|---|---|---|---|---|
| **Total of all processes** | **6.96E-03** | **1.12E-03** | **7.47E-04** | **3.77E-04** |
| | | | | |
| Heat, from hard coal | 6.47E-03 | 7.43E-04 | 2.57E-04 | 3.24E-07 |
| Electricity coal, ZA | 3.50E-04 | 2.69E-04 | 3.50E-04 | 2.69E-04 |
| Hard coal, at mine/EEU U | 7.85E-06 | 6.05E-06 | 7.85E-06 | 6.05E-06 |

### 4.4.4.4 Acidification

Figure 4.8 displays a similar dominance of better environmental performance of the hydrogen electricity options over the ethanol electricity options. EE still displays the worst performance compared to other options with 1.81 $x10^{-3}$ per MJ of electricity generated, with 62% due to use of coal for process heating as presented in Table 4.7 below.

Although coal is the biggest contributor, it does not display the same dominance as in the previous impact categories. Coal based electricity also contributes quite a sizeable amount for EE, with a 30% contribution to the total impact category despite its use in the production of ethanol being lower by a factor of 10 compared to coal used for process heating. The emissions in the combustion of ethanol electricity, especially $NO_x$ contributed about 8% to the overall acidification potential impact. The EE-HI displays a lower contribution as would be expected because it uses less coal for process heating; however the biggest contribution comes from coal based electricity emissions. These emissions contribute more than 70% of the overall emissions for this option. HE and HE-HI options also display a similar trend with the use of coal based electricity dominating. HE-HI still outscores all the other options in this impact category a result of self-sufficiency for process heating, the only associated coal impacts are due to electricity use, hence displays the best environmental performance.

**Table 4.7 : Major process contributions to Acidification Potential for the electricity options in kg $SO_2$ equivalence per MJ of electricity generated**

| Process | EE | HE | EE-HI | HE-HI |
|---|---|---|---|---|
| **Total of all processes** | **1.81E-03** | **6.72E-04** | **7.04E-04** | **5.43E-04** |
| | | | | |
| Heat, from hard coal | 1.12E-03 | 1.29E-04 | 4.46E-05 | 1.78E-06 |
| Electricity coal, ZA | 5.44E-04 | 4.19E-04 | 5.44E-04 | 4.19E-04 |
| EE emissions | 1.31E-04 | - | - | - |
| HE emissions | - | 1.15E-04 | - | - |
| EE-HI emissions | - | - | 1.05E-04 | - |
| HE-HI emissions | - | - | - | 1.15E-04 |
| Hard coal, mine | 2.30E-06 | 1.78E-06 | 2.30E-06 | 4.51E-07 |

**Table 4.8 : Substance contribution to Acidification Potential in kg $SO_2$ equivalence per MJ of electricity generated**

| Substance | EE | HE | EE-HI | HE-HI |
|---|---|---|---|---|
| **Total** | **1.81E-03** | **6.72E-04** | **7.04E-04** | **5.43E-04** |
| | | | | |
| Ammonia | 5.22E-06 | 9.02E-07 | 6.51E-07 | 3.56E-07 |
| Nitrogen oxides | 3.67E-04 | 2.04E-04 | 1.97E-04 | 1.84E-04 |
| Sulfur dioxide | 1.44E-03 | 4.67E-04 | 5.03E-04 | 3.59E-04 |
| Sulfur oxides | 4.57E-06 | - | - | - |

## Eutrophication

The Eutrophication Potential impact category as displayed in Figure 4.9 and 4.10 displays a different trend to the other impact categories that were dependent on the emissions from the use of coal. This impact category mainly accounts for the amount of organic matter and nutrients in the liquid effluent streams from the processes that are disposed to aquatic systems. The spent grain with water, stillage, is rich in such nutrients that have been concentrated due to the extraction of starch from maize grains. Because the contribution to this impact category is based on the effluent streams in the production of ethanol and hydrogen and not on the emissions associated with coal for process heat and electricity generation, the performances for electricity with and without integration are almost similar.

Although coal use for process heating also contributes to this category, the contribution is minimal as indicated in Table 4.9 and 4.10 which show both substance and process contributions; it is because of this minute contribution from coal that EE-HI shows a better performance than EE. For HE, this trend is not significant; the coal usage contribution to this impact category is so small that it is almost negligible in comparison to the production effluent that the options seem to

have the same performance. The HE options show a better performance by almost 60 % over the EE options, a factor which is in agreement with an assumption stated earlier, that the amount of the COD content in the hydrogen effluent (spent grain) is about half that of hydrogen, an additional improved performance is due to coal emissions for ethanol production. Hydrogen electricity still displays its dominance in better environmental performance as compared to that of ethanol – but is subject to the COD assumption made.

**Table 4.9 : Substances contribution to Eutrophication Potential in kg $PO_4$ equivalence per MJ of electricity generated**

| Substance | EE | HE | EE-HI | HE-HI |
|---|---|---|---|---|
| Total | 2.85E-03 | 9.90E-04 | 2.80E-03 | 9.84E-04 |
| | | | | |
| COD | 1.61E-03 | 5.47E-04 | 1.61E-03 | 5.47E-04 |
| Phosphorus, total | 8.58E-04 | 2.93E-04 | - | - |
| Nitrogen, total | 2.82E-04 | 9.61E-05 | - | - |
| Nitrogen oxides | 9.55E-05 | 5.31E-05 | 5.11E-05 | 4.78E-05 |
| Phosphate | 1.59E-06 | 3.83E-07 | 3.56E-07 | 2.35E-07 |

**Table 4.10 : Major process contribution to eutrophication potential for the electricity options per MJ of electricity in kg $PO_4$ equivalence per MJ of electricity generated**

| Process | EE | HE | EE-HI | HE-HI |
|---|---|---|---|---|
| **Total of all processes** | **2.85E-03** | **9.90E-04** | **2.80E-03** | **9.84E-04** |
| | | | | |
| Heat, from hard coal | 4.93E-05 | 5.67E-06 | 1.96E-06 | 6.64E-08 |
| Electricity coal, ZA | 2.25E-05 | 1.73E-05 | 2.25E-05 | 1.73E-05 |
| Ethanol production | 2.75E-03 | - | 2.75E-03 | - |
| Hydrogen production | - | 9.36E-04 | - | 9.36E-04 |
| EE emissions | 2.61E-05 | - | - | - |
| HE emissions | - | 2.99E-05 | - | - |
| EE-HI emissions | - | - | 2.61E-05 | - |
| HE-HI emissions | - | - | - | 2.99E-05 |



### 4.4.5 Comparing the results within impact categories for transport options

This section discusses the different impact assessment categories that were used to assess the inventory results for the transport options. Figure 4.9 below summarises the results, and the following subsections will discuss the individual impact categories and their contributing sub-processes.

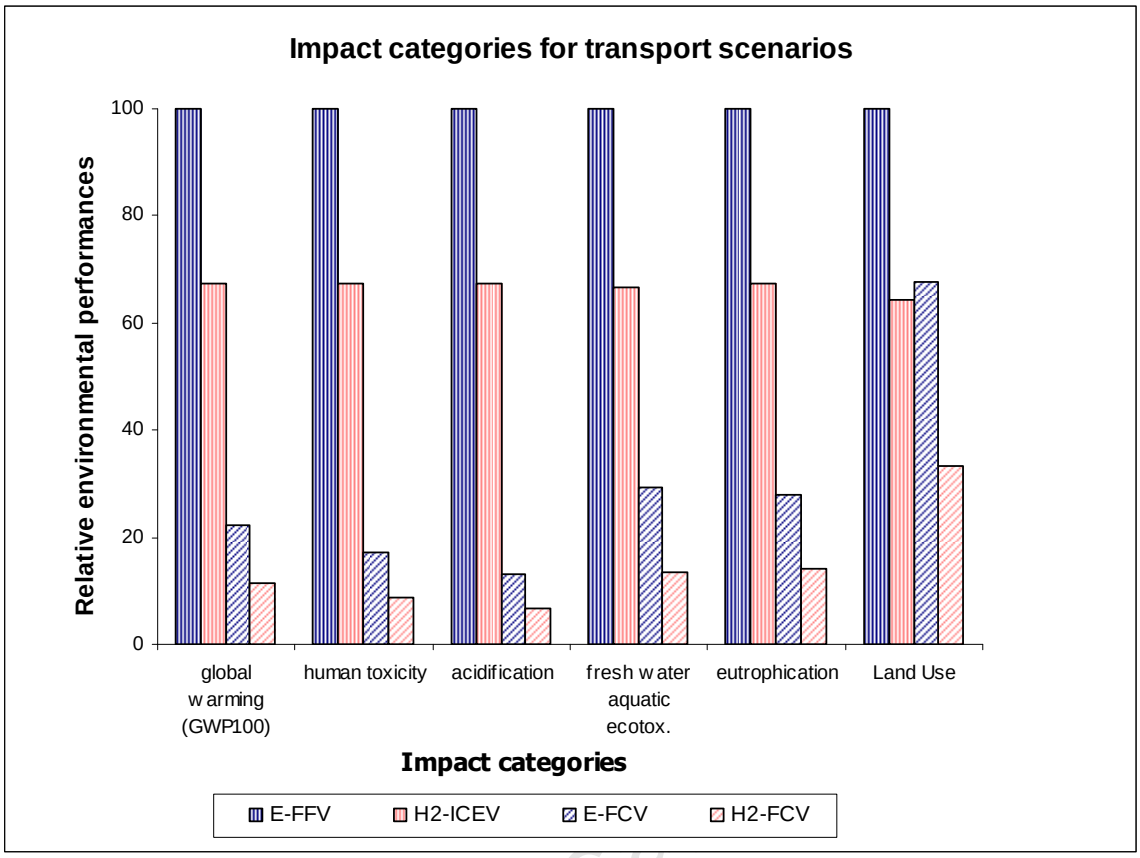


**Figure 4.9 : Comparison of environmental performances of transport options per kilometre driven**

### 4.4.5.1 Global warming potential

Hydrogen options are still showing their dominance, with the hydrogen transport options outperforming the ethanol transport options in all impact categories considered. The contribution to Global Warming Potential impact category results mainly from the production of bio-fuels ethanol and hydrogen as presented in Table 4.11. Carbon dioxide that it is released during the combustion of bioenergy fuels in combustion engines gives rise to what is termed biogenic emissions. These are emissions that do not contribute to the impact category because they are absorbed in the growth of maize, and hence represent short cycling of carbon. A similar trend to that of electricity options is evident here, with the major contributing processes being the ones that use fossil carbon in the bio-fuel production phase. E-FFV has the worst Global Warming impact performance followed by E-FCV, both these options have the same quantity of emissions associated with the production of ethanol; however the difference is due to the efficiency of the vehicles. Because of these differences in efficiencies of the vehicles, the E-FFV gives off more greenhouse gas emissions per km driven compared with the E-FCV. Table 4.11 presents this observation, for a kilometre driven on E-FFV, carbon dioxide equivalent emissions

from thermal heating in the production of ethanol is 0.214 kg, while it is 0.144 kg for ethanol fuel cell. This confirms the graphical representation on Figure 4.9, which shows the performance of the ethanol fuel cell vehicle to be superior by about 35%.

The better performance of the hydrogen options for this impact category can be attributed to two factors. The first one has been discussed extensively previously and is associated with less use of coal in the production of the hydrogen as opposed to the production of ethanol. The second factor is associated with the efficiencies of hydrogen vehicles in comparison with the ethanol vehicles. The issue of efficiency is also evident within the hydrogen vehicle options. The production of hydrogen incurs the same amount of emissions, however because the $H_2$-FCV is more efficient than $H_2$-ICEV the amount of emissions per kilometre differ. An example of carbon dioxide equiv. emissions for a kilometre driven for $H_2$-ICEV is $1.13 \times 10^{-1}$ compare to $5.85 \times 10^{-2}$ of $H_2$-FCV. This impact can be summed up as one that is more dependent on the efficiency more than on the quantity of fossil fuel used in bio-fuel production.

**Table 4.11 : Substance contribution to global warming potential in kg $CO_2$ for the transport options per kilometre driven**

| Substance | E-FFV | E-FCV | $H_2$-ICEV | $H_2$-FCV |
|---|---|---|---|---|
| **Total** | **2.20E-01** | **1.48E-01** | **4.85E-02** | **2.50E-02** |
| | | | | |
| Carbon dioxide, fossil | 2.05E-01 | 1.38E-01 | 4.46E-02 | 2.30E-02 |
| Methane, fossil | 1.52E-02 | 1.02E-02 | 4.02E-03 | 2.07E-03 |
| Dinitrogen monoxide | 8.28E-04 | 5.57E-04 | 1.96E-04 | 1.01E-04 |
| Carbon monoxide, fossil | 2.90E-04 | 1.95E-04 | 3.59E-05 | 1.85E-05 |
| Sulfur hexafluoride | 1.84E-05 | 1.24E-05 | 2.53E-06 | 1.30E-06 |

**Table 4.12 : Major process contributions to global warming potential in kg CO2 equivalence for transport options per a kilometre driven**

| Process | E-FFV | E-FCV | H2-ICEV | H-FCV |
|---|---|---|---|---|
| **Total of all processes** | **2.20E-01** | **1.48E-01** | **4.85E-02** | **2.50E-02** |
| | | | | |
| Heat, from hard coal | 1.67E-01 | 1.12E-01 | 1.54E-02 | 7.95E-03 |
| Electricity coal, ZA | 4.69E-02 | 3.16E-02 | 2.92E-02 | 1.50E-02 |
| Hard coal, at mine | 4.89E-03 | 3.29E-03 | 3.04E-03 | 1.57E-03 |
| Hardwood, allocation | 4.78E-04 | 3.22E-04 | 2.97E-04 | 1.53E-04 |

### 4.4.5.2 Human toxicity

This impact category as already mentioned explores the impact of harmful substances on humans. This impact category also mimics that of global warming

potential for the ethanol vehicle options. This can be explained using the same argument as above, which attributes the impact to the use of coal in the production of bio-ethanol, and the differences in performances between the E-FFV and the E-FCV to a better efficiency for the latter option. The hydrogen transport options show better performance here as in all the other cases studied. Table 4.12 shows that the contribution in this case is not only attributed to the coal used for process heating but coal based electricity contribute is more obvious for hydrogen options whose contribution is almost similar to that of process heating.

When the tail-pipe emissions are compared as shown in Table 4.13, for a kilometre driven, the tail-pipe emissions from the E-FFV is $1.290 \times 10^{-4}$ compared to $1.69 \times 10^{-5}$ for the $H_2$-ICEV; this can be associated with better vehicle efficiency. It can be concluded that in the Human Toxicity Potential impact category, the ethanol vehicle options were still outscored by hydrogen options; again coal use played a big role to the end performance.

**Table 4.13 : Major process contributions to human toxicity potential in kg 1,4-DB equivalence for the transport options per kilometre driven**

| Process | E-FFV | E-FCV | H2-ICEV | H-FCV |
|---|---|---|---|---|
| **Total of all processes** | **6.03E-02** | **4.05E-02** | **1.04E-02** | **5.27E-03** |
| | | | | |
| Heat from hard coal | 5.14E-02 | 3.46E-02 | 4.76E-03 | 2.45E-03 |
| Electricity coal, ZA | 8.14E-03 | 5.47E-03 | 5.06E-03 | 2.61E-03 |
| Hard coal,mine | 9.46E-05 | 6.37E-05 | 5.88E-05 | 3.03E-05 |
| E-FFV emissions | 1.29E-04 | - | - | - |
| E-FCV emissions | - | 7.07E-05 | - | - |
| H2-ICEV emissions | - | - | 1.69E-04 | - |
| H-FCV emissions | - | - | - | 1.67E-05 |



### 4.4.5.3 Fresh water aquatic eco-toxicity

This subsection is a continuation of sub-section 4.4.4.3 for this impact category, with the focus geared towards the four transport options. This impact category mimics that of global warming potential, as can be seen in Figure 4.9. There are only two main contributing processes to this impact category, these are process heating using coal and coal based electricity as shown in Table 4.13 below. Tail-pipe emissions contributions are minute compared to the ones presented in the table below; hence they are left out.

Efficiency of the vehicles has emerged as a performance factor right through the previous impact categories; it is seen to play a role here as well. Since the same amount of fossil fuel would be used for the production of the transport fuels and that the impact category is not dependent on the tail-pipe emissions, the only aspect that can be attributed to the difference in emissions per kilometre driven can be associated with the vehicle efficiencies. Fuel cell vehicles are more efficient than internal combustion vehicles; hence show better performance in the impact category. Hydrogen options are more efficient and use less fossil fuel than ethanol in their production phase hence show better environmental performance for this category.

**Table 4.14: Major processes contributions to fresh water aquatic eco-toxicity potential in kg 1,4-DB equivalence for the transport options per kilometre driven**

| Process | E-FFV | E-FCV | H2-ICEV | H-FCV |
|---|---|---|---|---|
| **Total of all processes** | **7.66E-03** | **5.15E-03** | **9.94E-04** | **5.13E-04** |
| | | | | |
| Heat from hard coal | 7.12E-03 | 4.79E-03 | 6.59E-04 | 3.40E-04 |
| Electricity coal, ZA | 3.85E-04 | 2.59E-04 | 2.39E-04 | 1.23E-04 |
| Hard coal | 8.64E-06 | 5.81E-06 | 5.37E-06 | 2.77E-06 |



### 4.4.5.4 Acidification potential

This section discusses the acidification potential impact of the four vehicle options, as presented in Figure 4.9 above and Table 4.15 below. Acidification is one impact category that it is tied in with the usage of coal due to sulphur dioxide emissions given off during coal combustion, thus it is not surprising for this impact category to show a similar trend to that shown for global warming potential. Table 4.15 shows this aspect that the most contributing process to acidification is the use of coal used for process heating and coal based electricity in the production process of transport fuel. Tail-pipe emissions have a small contribution to the overall impact presented here per kilometre driven. The impact category can be summarised as follows, fuel cell vehicles are more efficient and thus give smaller emissions than ICE vehicles as shown in the previous impact categories. Hydrogen vehicles still outperform their ethanol counterparts, partly due to less coal use in the hydrogen production fuel and partly due to better vehicles efficiencies.

**Table 4.15: Major processes' contribution to acidification potential in kg $SO_2$ equivalence for the transport options per a kilometre driven**

| Process | E-FFV | E-FCV | H2-ICEV | H-FCV |
|---|---|---|---|---|
| **Total of all processes** | **1.89E-03** | **1.26E-03** | **5.57E-04** | **2.55E-04** |
| | | | | |
| Heat from hard coal | 1.24E-03 | 8.31E-04 | 1.14E-04 | 5.90E-05 |
| Electricity coal, ZA | 5.98E-04 | 4.03E-04 | 3.72E-04 | 1.92E-04 |
| Hard coal | 2.54E-06 | 1.71E-06 | 1.58E-06 | 8.12E-07 |
| E-FFV emissions | 4.75E-05 | - | - | - |
| E-FCV emissions | - | 2.25E-05 | - | - |
| H2-ICEV emissions | - | - | 6.36E-05 | - |
| H-FCV emissions | - | - | - | - |

### 4.4.5.5 Eutrophication

This is one impact category whose primary dependence is not on the use of coal, rather on the amount the organic material in the process effluent streams, mostly reported in the chemical oxygen demand (COD) of the effluent streams as is the case in this study. The performance of the vehicle options is shown in Figure 4.9 and the contributing processes are shown in Table 4.16 below. As observed, in table 4.16 ethanol and hydrogen production processes are the biggest contributors to this category, a consequence of relatively high COD in the process effluent. Similar quantities and concentration of stillage are given off for the two ethanol vehicle options while similar quantities and concentration for hydrogen vehicle options are also disposed off. However, because of the difference in efficiencies in the vehicle types the relative contributions to eutrophication per kilometre driven were different. The fuel cell vehicles had better performance as the more efficient vehicles within the similar fuel type, while once again the hydrogen vehicles out-performed the ethanol ones mostly due an assumption made.

**Table 4.16: Major processes' contribution to eutrophication potential in kg $PO_4$ equivalence for transport options per kilometre driven**

| Process | E-FFV | E-FCV | H2-ICEV | H-FCV |
|---|---|---|---|---|
| **Total of all processes** | 3.11E-03 | 2.09E-03 | 8.68E-04 | 4.39E-04 |
| | | | | |
| Heat from hard coal | 5.43E-05 | 3.65E-05 | 5.03E-06 | 2.59E-06 |
| Electricity coal, ZA | 2.47E-05 | 1.66E-05 | 1.54E-05 | 7.92E-06 |
| Ethanol production | 3.02E-03 | 2.03E-03 | - | - |
| Hydrogen production | - | - | 8.30E-04 | 4.28E-04 |
| E-FFV emissions | 1.23E-05 | - | - | - |
| E-FCV emissions | - | 5.85E-06 | - | - |
| H2-ICEV emissions | - | - | 1.65E-05 | - |
| H-FCV emissions | - | - | - | - |

## *4.5 Discussion of the expanded systems*

This section, like the previous sections discusses the different impact categories used to evaluate the inventory results, however for options with expanded functionality.

Table 4.17 and Figure 4.10 below present the contribution of different fuels to the expanded systems. One of the goals of the study was to determine the best way to utilise maize for energy products by expanding the system boundaries as recommended by the ISO, so that the systems with different outputs could be compared directly. The impact categories that are studied, the tools used to generate data, and methodologies used for the impact categories here are as presented previously in Chapter 3 and Section 4.4.

The results in this section have been presented in graphical and tabular form, presenting the contributions of different sub-processes within a particular system.



### 4.5.1 The procedure of system expansion

The generated scenarios were expanded as outlined in Section 3.4, and the table below shows the primary fossil contributions for the 8 industrial options. The tabulated data comprised an LCI which was modelled in SimaPro version 7. The results of the LCA for the expanded options are presented in the subsequent sections.

**Table 4.17: Inventory summary for the 8 industrial options after system boundary expansion**

| Scenarios | | EE | HE | EE-HI | HE-HI | E-FFV | H2 ICEV | E-FCV | H2-FCV |
|---|---|---|---|---|---|---|---|---|---|
| Products | Units | | | | | | | | |
| | | | | | | | | | |
| Maize electricity | kWh | 3.14E+03 | 4.06E+03 | 3.14E+03 | 4.06E+03 | 0 | 0 | 0 | 0 |
| Coal used for maize electricity (heat) and (electricity) | MJ | 2.33E+04 | 2.47E+03 | 5.24E+02 | 0.00E+00 | 0 | 0 | 0 | 0 |
| | kWh | 7.00E+02 | 7.00E+02 | 7.00E+02 | 7.00E+02 | 0 | 0 | 0 | 0 |
| | | | | | | | | | |
| Maize Transport | km | 0 | 0 | 0 | 0 | 1.07E+04 | 1.66E+04 | 1.59E+04 | 3.22E+04 |
| Coal used for maize transport (heat) and electricity | MJ | 0 | 0 | 0 | 0 | 2.33E+04 | 2.47E+03 | 2.33E+04 | 2.47E+03 |
| | kWh | 0 | 0 | 0 | 0 | 7.00E+02 | 7.00E+02 | 7.00E+02 | 7.00E+02 |
| | | | | | | | | | |
| Coal based electricty added for system expansion | kWh | 9.22E+02 | 0 | 9.22E+02 | 0 | 4.06E+03 | 4.06E+03 | 4.06E+03 | 4.06E+03 |
| Amount of coal used to generate coal electricity | kg | 4.37E+02 | 0 | 4.37E+02 | 0 | 1.93E+03 | 1.93E+03 | 1.93E+03 | 1.93E+03 |
| Amount of energy inherent in coal for electricity | MJ | 1.01E+04 | 0 | 1.01E+04 | 0 | 4.43E+04 | 4.43E+04 | 4.43E+04 | 4.43E+04 |
| Gasoline added for system expansion | km | 3.22E+04 | 3.22E+04 | 3.22E+04 | 3.22E+04 | 2.15E+04 | 1.55E+04 | 1.63E+04 | 0 |
| Gasoline used to achieve the mileage | kg | 2.23E+03 | 2.23E+03 | 2.23E+03 | 2.23E+03 | 1.49E+03 | 1.08E+03 | 1.13E+03 | 0 |
| | MJ | 9.69E+04 | 9.69E+04 | 9.69E+04 | 9.69E+04 | 6.46E+04 | 4.68E+04 | 4.91E+04 | 0 |



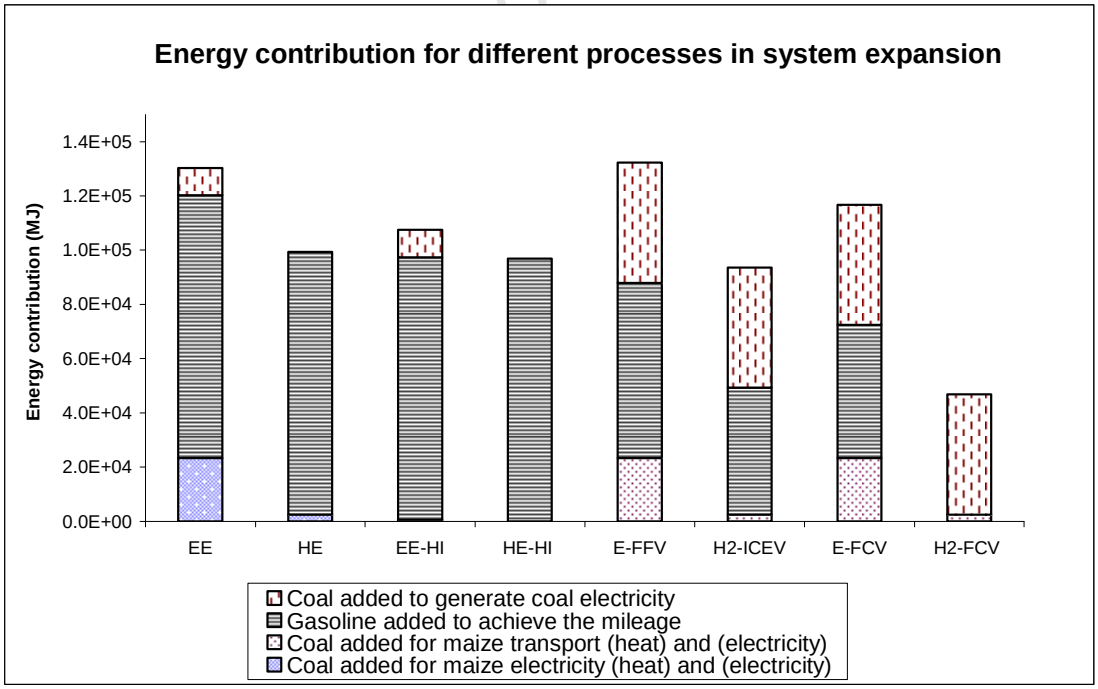


**Figure 4.10 : Primary fossil energy needed to deliver extended system functionality of 4060 kWh of electricity and 32200 km (passenger car) delivered from maize grown on 1 hectare of land**

### 4.5.2 Dominance of the hydrogen options

Figure 4.11 below presents the environmental performance of the 8 expanded options based on the 5 impact categories selected and discussed in Chapter 3. The results of the expanded systems show a clear dominance of the hydrogen options in most of the selected impact categories as was the case before the systems were expanded. The reasons for this are found in dependence on coal use and better process efficiency, and are well discussed in the previous sections. Although the hydrogen options dominate in most of the impact categories, their impact categories performances vary depending on different options and impact category. The following sections will discuss the individual contributions that result in different impact categories performances.

### 4.5.3 Replacing the "dirtier" fuel

From Figure 4.11, it can be seen that the electricity options show better environmental performance than the corresponding transport options in all impact categories with the exception of global warming potential where the difference is marginal. Replacing the dirtiest fuel (in this case, coal-based electricity) with the available renewable energy shows the best environmental benefits when the systems are expanded. Refineries, and motor vehicles, unlike coal-based electricity power stations, usually have pollution control devices (e.g. wet scrubbers or catalytic converters) in place to cleanse their air emissions; this reduces the level of pollutants that would otherwise be emitted directly to the environment. On the other hand, South African coal-based electricity does not have such advanced technologies in place, making it one of the "dirtiest" thermal electricity generation processes.

The results obtained here resonate with a general wisdom emerging from LCA literature, viz. that limited renewable energy should always be targeted at replacing the "dirtiest fuel in the system" (Finnveden, 2005). In this case it is coal-based electricity, as pointed out in chapter 1 where the study by von Blottnitz (2006) was cited, comparing South African coal based electricity with that of 16 European countries. It was found that South Africa has the highest emissions of $SO_x$, $NO_x$ and particulates per kWh of electricity produced of all the countries it was compared to. Renewable energy based electricity options, to which minor or no additions of coal-based electricity were made upon system expansion hence show better performance in the impact categories that are directly impacted by those emissions, such as

Human Toxicity, Acidification and Fresh Water Aquatic Toxicity. The global warming potential performance is almost at par with the transport ones because the fossil-based transport fuels also emit considerable amounts of greenhouse gases in their production and use.

### 4.5.4 The effect of heat integration

Heat integration into power generation options shows the best environmental performance in all the impact categories for the individual fuels but global warming potential performance. This outlier performance was investigated by carrying out a basic mass balance for carbon dioxide equivalence emissions, the greenhouse contributor to global warming potential for HE with H2-ICEV options[2]. When systems were expanded a certain amount of gasoline (life cycle) was added to the electricity option while coal based electricity (life cycle) was added to the transport option. It turns out that the carbon dioxide equivalent emissions associated with gasoline exceed those of coal-based electricity added to the transport option due to larger quantities added. However, as mentioned in section 4.5.3 there is better pollutants management and reduction of other emissions such as $SO_x$, $NO_x$ and particulates at the refinery and in the passenger vehicle than in a coal-based power plant. The other impact categories are based on these emissions; hence a better performance of the electricity options compared to transport options is displayed. HE-HI emerges the best option, for the reasons that have been outlined in the previous sections.

### 4.5.5 The use of fuel cell technology

The use of fuel cell technology generally displays a marginal improvement in the environmental performance due to improved technology efficiency of the fuel cell vehicles in comparison with the internal combustion engine vehicles for options with expanded functionality, although when compared before system boundary expansion, a better performance is seen as shown in Figure 4.9. The one impact category that shows a distinct improvement is the global warming potential again due to the reasons discussed in Section 4.5.4 that results from the greenhouse gas emissions for gasoline life cycle exceeding those of coal-based electricity for expanded systems. The other impact categories show just a slight improvement in the performance; this is due to the addition of equal amounts of coal-based electricity that has high emissions of $SO_x$, $NO_x$ and particulates which brings overall

[2] Appendix A5

emissions associated with the options to the be similar when systems are brought to the same level of comparison by system boundary expansion.

The subsequent subsections will now explore the individual impact categories in more detail.

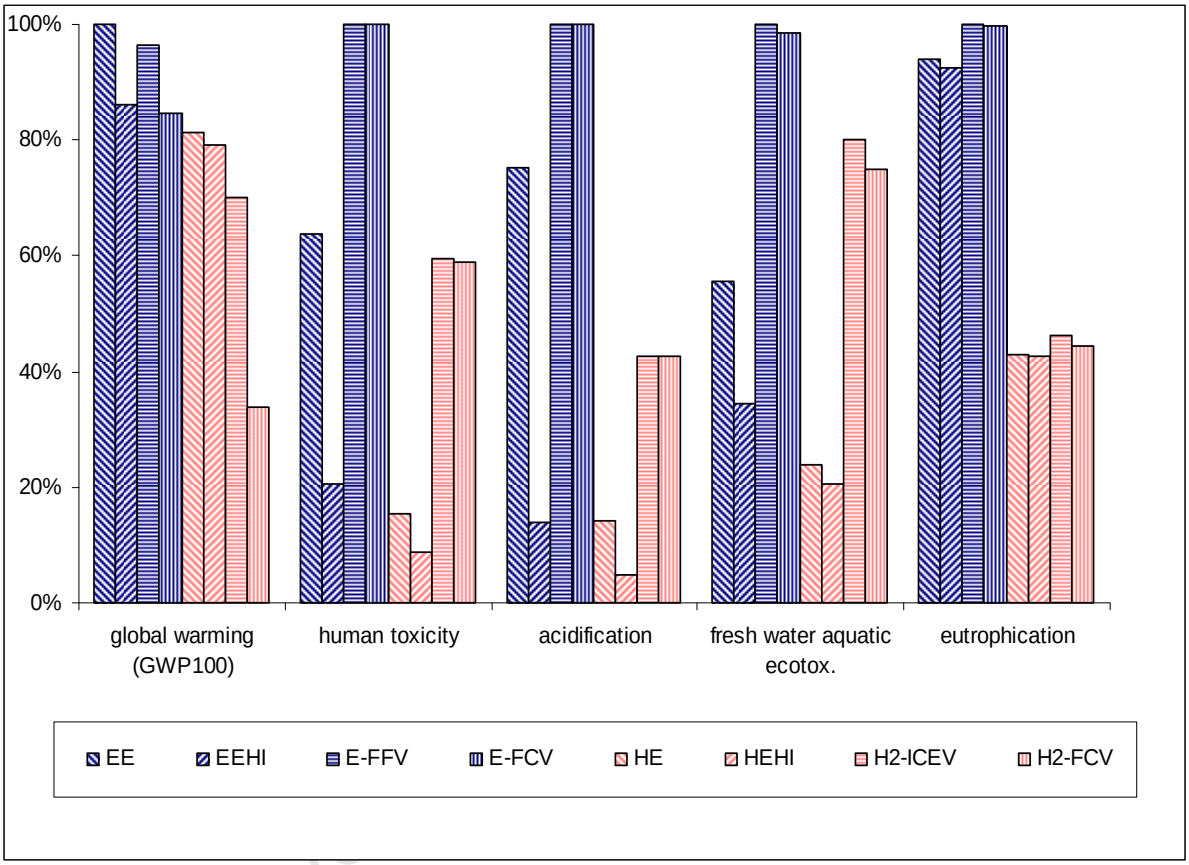


**Figure 4.11: Relative comparison of the impact categories for the 8 scenarios with expanded functionality (basis 1 ha)**

## 4.5.6 Analysis of the individual impact categories

This section takes an extensive look at the individual contributions of the expanded options to the impact categories for the expanded scenarios.

### 4.5.6.1 Global Warming Potential

**Table 4.18: Process contribution to global warming potential for systems with extended functionality in kg $CO_2$ equivalence**

| Process | EE | EE-HI | E-FFV | E-FCV | HE | HE-HI | H2-ICEV | H2-FCV |
|---|---|---|---|---|---|---|---|---|
| **Total of all processes** | **1.05E-01** | **9.02E-02** | **1.01E-01** | **8.86E-02** | **8.54E-02** | **8.31E-02** | **7.34E-02** | **3.56E-02** |
| | | | | | | | | |
| EE gasoline emissions | 7.82E-02 | - | - | - | - | - | - | - |
| EE-HI gasoline emissions | - | 7.82E-02 | - | - | - | - | - | - |
| E-FFV gasoline emissions | - | - | 5.16E-02 | - | - | - | - | - |
| E-FCV gasoline emissions | - | - | - | 3.92E-02 | - | - | - | - |
| HE gasoline emissions | - | - | - | | 7.82E-02 | - | - | - |
| HE-HI gasoline emissions | - | - | - | | - | 7.82E-02 | - | - |
| H2-ICEV gasoline emissions | - | - | - | | - | - | 3.78E-02 | - |
| H2-FCV gasoline emissions | - | - | - | | - | - | - | - |
| Heat from hard coal | 1.53E-02 | 6.06E-04 | 1.59E-02 | 1.59E-02 | 2.27E-03 | 3.05E-05 | 2.29E-03 | 2.29E-03 |
| Electricity coal, ZA | 9.99E-03 | 9.99E-03 | 2.95E-02 | 2.95E-02 | 4.28E-03 | 4.28E-03 | 2.94E-02 | 2.94E-02 |
| Hard coal, at mine | 1.04E-03 | 1.04E-03 | 3.08E-03 | 3.08E-03 | 4.46E-04 | 4.46E-04 | 3.06E-03 | 3.06E-03 |
| Hardwood, allocation | 1.02E-04 | 1.02E-04 | 3.01E-04 | 3.01E-04 | 4.37E-05 | 3.52E-05 | 3.00E-04 | 3.00E-04 |

***Electricity scenarios:***

Most carbon dioxide equivalent emissions for the expanded systems are associated with the addition of gasoline to the seven options except the most efficient $H_2$-FCV option that returns a mileage of 32200 km. The life cycle of gasoline was modelled in GREET version 2.7 (Argonne Laboratory, 2006), and the associated emissions modelled in the LCA software, SimaPro version 7. Coal-based electricity greenhouse gas emissions that result from electricity addition to the electricity options when system boundaries are expanded are small compared to gasoline associated emissions from the addition of gasoline. Because the same amount of gasoline is added to the electricity options the same amount of emissions related to gasoline and additional coal-based electricity (in the case of ethanol options) are obtained, as seen in Table 4.18. The difference in their performance results from varying quantities of coal used in their production. The EE option has the highest contribution as it utilises the most coal in its production, utilising both coal to meet its thermal and electricity needs, thus the resulting emissions from coal based electricity are higher than EE-HI solely due replaced coal input due to heat integration in the production phase. HE has better performance than both the ethanol electricity options because of the lower use of coal and better energy yield from the reference flow. The difference is marginal because gasoline greenhouse gas emissions are dominant for the electricity options. HE-HI has the best results of all

the electricity options because heat integration replaces all its thermal requirements, resulting in the contribution being just from coal-based electricity used in the production phase and gasoline greenhouse gas emissions after system boundary expansion.

### *Transport Scenarios*

The amount of gasoline added when the system boundaries were expanded for the transport options depended on the vehicle efficiency, the more efficient the option is, the closer it is to the maximum amount of kilometres that can be driven on a maize energy product hence the less gasoline needed to be added to an option for comparison of options with extended functionality. E-FFV is the least efficient of the transport options, hence had the highest greenhouse gas emissions associated with the addition of gasoline. The same amount of coal-based electricity was added to all the non-electricity generating options. However, E-FFV and E-FCV have the highest emissions associated with coal-based electricity because in addition to that added for system expansion they had similar thermal requirements for the production of ethanol fuel. The hydrogen transport options show better GHG performance because of better fuel production efficiency and less dependence on coal, with $H_2$-ICEV also requiring less gasoline added to it for system expansion and hence resulting in less overall greenhouse gas emissions. The $H_2$-FCV has the best performance of all the transport options mainly because gasoline was not added, as the most efficient vehicle option that delivers the most mileage (32200 km). The green house emissions for $H_2$-FCV are only due to the addition of coal-based electricity to the option and coal in the production of the fuel.

Global warming sees transport options having a better performance in global warming potential compared to the corresponding electricity options, a result of overall carbon dioxide emissions discussed in Section 4.5.3.

### 4.5.6.2 Acidification

**Table 4.19 : Process contribution to acidification potential for systems with expanded functionality in kg $SO_2$ equivalence**

| Process | EE | EE-HI | E-FFV | E-FCV | HE | HE-HI | H2-ICEV | H2-FCV |
|---|---|---|---|---|---|---|---|---|
| **Total of all processes** | **2.96E-04** | **1.84E-04** | **5.33E-04** | **5.26E-04** | **1.27E-04** | **1.10E-04** | **4.28E-04** | **3.99E-04** |
| | | | | | | | | |
| Electricity coal, ZA | 1.27E-04 | 1.27E-04 | 3.77E-04 | 3.77E-04 | 5.46E-05 | 5.46E-05 | 3.75E-04 | 3.75E-04 |
| Heat from hard coal | 1.13E-04 | 4.50E-06 | 1.18E-04 | 1.18E-04 | 1.68E-05 | 2.31E-07 | 1.70E-05 | 1.70E-05 |
| EE gasoline emissions | 3.95E-05 | - | - | - | - | - | - | - |
| EE-HI gasoline emissions | - | 3.93E-05 | - | - | - | - | - | - |
| E-FFV gasoline emissions | - | - | 2.63E-05 | - | - | - | - | - |
| E-FCV gasoline emissions | - | - | - | 2.00E-05 | - | - | - | - |
| HE gasoline emissions | - | - | - | - | 3.95E-05 | - | - | - |
| HE-HI gasoline emissions | - | - | - | - | - | 3.95E-05 | - | - |
| H2-ICEV gasoline emissions | - | - | - | - | - | - | 1.90E-05 | - |
| H2-FCV gasoline emissions | - | - | - | - | - | - | - | - |
| EE emissons | 1.32E-05 | - | - | - | - | - | - | - |
| HE emissons | - | - | - | - | 1.50E-05 | - | - | - |
| EE-HI emissons | - | 1.06E-05 | - | - | - | - | - | - |
| HE-HI emissons | - | - | - | - | - | 1.50E-05 | - | - |
| E-FFV emissons | - | - | 4.54E-06 | - | - | - | - | - |
| E-FCV emissons | - | - | - | 3.20E-06 | - | - | - | - |
| H2-ICEV emissons | - | - | - | - | - | - | 9.42E-06 | - |
| H2-FCV emissons | - | - | - | - | - | - | - | - |



***Electricity scenarios***

The biggest contribution for the electricity scenarios in this impact category results from coal usage for either process heating or coal-based electricity. The emissions associated with gasoline added when system boundaries were expanded are similar (and small) for all the electricity options, as expected. Also, similar (and dominant) coal-based electricity emissions are due to similar amounts of coal-based electricity added to the ethanol electricity options, as can be observed in Table 4.19. Although the amount of gasoline added to EE when systems were expanded is by far more than coal-based electricity as calculated and presented in Table 4.16, $SO_2$ equiv. emissions from the coal-based electricity emissions still dominate: this observation concurs with the fact that refineries have better control measures than the coal based power stations for $SO_2$ emissions among others. EE-HI and HE-HI outperform the corresponding EE and HE because of less use of coal in the generation of the individual fuels hence the associated $SO_2$ emissions. Hydrogen electricity options outperform the ethanol ones for this impact category as can be seen in Table 4.19 above.

### *Transport options*

Similar quantities of coal-based electricity are added to all the transport options when systems are expanded, hence similar $SO_2$ equiv. associated emissions. As in the previous subsection, the $SO_2$ equiv. emissions from coal-based electricity exceeds that of gasoline despite a higher tonnage because emissions from the coal-based power plants are dirtier for reasons already outlined in Section 4.5.3. The second biggest contributor comes from addition of gasoline, whose addition is efficiency dependent, the more efficient the vehicle is, the less the amount of gasoline that needs to be added to the option, hence the less the $SO_2$ equiv emissions. E-FFV has the highest $SO_2$ equiv. emissions compared to all other transport options as it also uses the highest coal based electricity and coal for process heating together with E-FCV, however it is the least efficient of all the vehicles it and gets the most gasoline added gasoline added to it, presenting an overall poorer performance. $H_2$-FCV has the best performance as the most efficient vehicle, with no addition of gasoline and less intensive use of coal.

The electricity options outscore the performance of the transport options for acidification, a result of a replacement of the dirty fuel with a cleaner one having the best environmental gains as discussed in Section 4.5.3.

### 4.5.6.3 Human toxicity

**Table 4.20 : Processes contribution to human toxicity potential for the systems with expanded functionality in kg 1,4-DB equivalence**

| Process | EE | EE-HI | E-FFV | E-FCV | HE | HE-HI | H2-ICEV | H2-FCV |
|---|---|---|---|---|---|---|---|---|
| **Total of all processes** | **6.67E-03** | **2.14E-03** | **1.05E-02** | **1.05E-02** | **1.60E-03** | **9.05E-04** | **6.23E-03** | **6.17E-03** |
| | | | | | | | | |
| Heat from hard coal | 4.73E-03 | 1.87E-04 | 4.97E-03 | 4.91E-03 | 7.09E-04 | 8.64E-06 | 1.45E-03 | 7.51E-04 |
| Electricity coal, ZA | 1.73E-03 | 1.73E-03 | 5.12E-03 | 5.12E-03 | 7.43E-04 | 7.43E-04 | 5.09E-03 | 5.09E-03 |
| EE gasoline emissions | 7.19E-05 | - | - | - | - | - | - | - |
| EE-HI gasoline emissions | - | 7.17E-05 | - | - | - | - | - | - |
| E-FFV gasoline emissions | - | - | 4.80E-05 | - | - | - | - | - |
| E-FCV gasoline emissions | - | - | - | 3.65E-05 | - | - | - | - |
| HE gasoline emissions | - | - | - | - | 7.19E-05 | - | - | - |
| HE-HI gasoline emissions | - | - | - | - | - | 7.19E-05 | - | - |
| H2-ICEV gasoline emissions | - | - | - | - | - | - | 3.47E-05 | - |
| H2-FCV gasoline emissions | - | - | - | - | - | - | - | - |
| EE emissions | 2.73E-05 | - | - | - | - | - | - | - |
| HE emissions | - | - | - | - | 3.60E-05 | - | - | - |
| EE-HI emissions | - | 2.48E-05 | - | - | - | - | - | - |
| HE-HI emissions | - | - | - | - | - | 3.60E-05 | - | - |
| E-FFV emissions | - | - | 1.23E-05 | - | - | - | - | - |
| E-FCV emissions | - | - | - | 1.00E-05 | - | - | - | - |
| H2-ICEV emissions | - | - | - | - | - | - | 2.51E-05 | - |
| H2-FCV | - | - | - | - | - | - | - | - |



***Electricity options***

The trend observed with Human Toxicity Potential presented here is similar to that of Acidification Potential discussed above; the emissions associated with gasoline are similar for all electricity options, hence have similar 1,4-DB equivalence emissions as observed in Table 4.19. Coal use for process heating and coal-based electricity have the highest emissions compared to gasoline related emissions except for HE-HI which does not use of coal for process heat, utilising only coal based-electricity in the production of HE-HI.

***Transport options***

The emissions from coal-based electricity added to the options when systems were expanded have a significant contribution to human toxicity. Table 4.19 shows E-FFV to have the worst performance; because it uses coal for fuel production in addition to system expansion and is also the least efficient of the vehicle options resulting in more gasoline related emissions compared to others. $H_2$ FCV is the most efficient vehicle and uses the least amount of coal for production hence it has the best environmental performance.

This impact category is dependent on the coal combustion emissions, and since it has already been discussed that coal is a dirtier fuel than gasoline, the electricity options that replace the dirtiest fuel outscore the transport performance for human toxicity.

### 4.5.6.4 Fresh water aquatic eco-toxicity

**Table 4.21 : Process contribution to fresh water aquatic eco-toxicity potential for systems with extended functionality in kg 1,4-DB equivalence**

| Process | EE | EE-HI | E-FFV | E-FCV | HE | HE-HI | H2-ICEV | H2-FCV |
|---|---|---|---|---|---|---|---|---|
| **Total of all processes** | **7.68E-04** | **1.41E-04** | **1.02E-03** | **1.02E-03** | **1.46E-04** | **4.92E-05** | **4.35E-04** | **4.35E-04** |
| | | | | | | | | |
| Heat from hard coal | 6.53E-04 | 2.59E-05 | 6.80E-04 | 6.80E-04 | 9.69E-05 | - | 9.77E-05 | 9.77E-05 |
| Electricity coal, ZA | 8.19E-05 | 8.19E-05 | 2.42E-04 | 2.42E-04 | 3.51E-05 | 3.51E-05 | 2.41E-04 | 2.41E-04 |
| Hard coal, mine | 1.84E-06 | 1.84E-06 | 5.44E-06 | 5.44E-06 | 7.89E-07 | 7.89E-07 | 5.41E-06 | 5.41E-06 |

***Electricity options***

There were negligible contributions from gasoline life cycle emissions for fresh water aquatic eco-toxicity. Emissions from coal used for process heating and coal-based electricity are the biggest contributors to this impact category. EE has the worst performance of all the options because of similar well-discussed reasons presented in above sections, while HE-HI has the best performance.

***Transport emissions***

Similar amounts of coal-based electricity are added to the transport systems upon expansion, resulting in similar coal-based emissions for all the vehicle options. Since this category seems to be linked with coal use, at the risk of repeating what has already been discussed, similar implications as associated with acidification and human toxicity can be suspected here.

### 4.5.6.5 Eutrophication

**Table 4.22: Process contribution to eutrophication potential for systems with expanded functionality in kg $PO_4$ equivalence**

| Process | EE | EE-HI | E-FFV | E-FCV | HE | HE-HI | H2-ICEV | H2-FCV |
|---|---|---|---|---|---|---|---|---|
| **Total of all processes** | **2.97E-04** | **2.92E-04** | **3.16E-04** | **3.14E-04** | **1.35E-04** | **1.35E-04** | **1.46E-04** | **1.40E-04** |
| | | | | | | | | |
| Ethanol production | 2.77E-04 | 2.77E-04 | 2.89E-04 | 2.89E-04 | - | | | |
| Hydrogen production | - | - | - | - | 1.22E-04 | 1.22E-04 | 1.23E-04 | 1.23E-04 |
| Electricity coal, ZA | 5.27E-06 | 5.27E-06 | 1.56E-05 | 1.56E-05 | 2.26E-06 | 2.26E-06 | 1.55E-05 | 1.55E-05 |
| Heat from hard coal | 4.98E-06 | 1.98E-07 | 5.19E-06 | 5.19E-06 | 7.39E-07 | - | 7.45E-07 | 7.45E-07 |
| EE gasoline emissions | 6.39E-06 | - | - | - | - | - | - | - |
| EE-HI gasoline emissions | - | 6.36E-06 | - | - | - | - | - | - |
| E-FFV gasoline emissions | - | - | 4.26E-06 | - | - | - | - | - |
| E-FCV gasoline emissions | - | - | - | 3.24E-06 | | - | - | - |
| HE gasoline emissions | - | - | - | - | 6.39E-06 | - | - | - |
| HE-HI gasoline emissions | - | - | - | - | - | 6.39E-06 | - | - |
| H2-ICEV gasoline emissions | - | - | - | - | - | - | 3.08E-06 | - |
| H2-FCV gasoline emissions | - | - | - | - | - | - | - | - |
| EE emissons | 2.63E-06 | - | - | - | - | - | - | - |
| HE emissons | - | - | - | - | 3.90E-06 | - | - | - |
| EE-HI emissons | - | 2.63E-06 | - | - | - | - | - | - |
| HE-HI emissons | - | - | | - | - | 3.90E-06 | - | - |
| E-FFV emissons | - | - | 1.17E-06 | - | - | - | - | - |
| E-FCV emissons | - | - | - | 8.31E-07 | - | - | - | - |
| H2-ICEV emissons | - | - | - | - | - | - | 2.45E-06 | - |
| H2-FCV emissons | - | - | - | - | - | - | - | - |



***Electricity options***

This is one category that does not rely heavily on fossil fuel based emissions, but on the nutrients and organic matter present in effluent or process waste streams. Table 4.22 shows how minimal the contributions of gasoline emissions, coal-based electricity and coal used for heating purposes are. The major contribution comes from the nutrient effluent produced in the production of either ethanol or hydrogen. The ethanol options have a higher impact - a consequence of an assumption made earlier in Chapter 3. The hydrogen options show better environmental performance, and since they have exactly the same effluent their performances are similar.

***Transport options***

The ethanol and hydrogen transport options have almost similar performances for similar reasons discussed above resulting from the effect of effluent in the production phase; the slight differences shown are due to small contributions from fossil fuels. Hydrogen transport options display a better performance than the ethanol options, as a result of the assumptions made in chapter 3 on stillage composition.

The electricity options still exhibit a better performance than the transport options, this difference is traced to coal-based electricity that is added to transport options. The addition of coal-based electricity has the associated emissions that also contribute to Eutrophication Potential, although the difference between the electricity

## *4.6 LCA Interpretation*

This section describes the final phase of the life cycle assessment procedure. The results of life cycle inventory (LCI) and life cycle impact assessment (LCIA) are summarised and discussed as a basis for conclusions and recommendations in line with the goal and scope, as recommended in ISO 14043.

The goal of the study was to primarily analyse the environmental performance of the two maize-derived energy products; ethanol and hydrogen with each other. Their performance was assessed by the impact they have on the environment when used to generate peak power and when used as transport fuel. First significant issues based on the results of LCI and LCIA will be identified and discussed, and an evaluation that considers completeness and conclusions will be made.

### 4.6.1 Identification of significant issues

LCI and LCIA analyses showed that the use of coal for either thermal purposes or electricity had the most negative environmental impacts for the options considered in the study. It was established that the more the quantity of coal used for process heat in any given electricity option, the worse the environmental impact, thus the option that made use of the highest amount of coal had the most adverse environmental impacts. The use of coal was identified as an issue of concern because of the associated gaseous emissions. Table 4.23 summarises coal usage for transport options and some of the influential emissions to the impact categories.

The highlighted flows in Table 4.23 represent the highest flow of all the electricity options. As discussed earlier, hydrogen electricity is more environmentally attractive than ethanol electricity. Table 4.24 quantifies the total emissions of the impact categories for power generation options, and EE as highlighted, has the worst environmental impacts while HE-HI is the best performing option for well discussed reasons, all associated with use of coal and the efficiency of the process.

**Table 4.23 : A summary of coal usage and overall major emissions for electricity options**

| LCI input/output | EE | EE-HI | HE | HE-HI |
|---|---|---|---|---|
| | kg | kg | kg | kg |
| Hard coal used for thermal requirements and coal based electricity | **1.34E+03** | 3.53E+02 | 4.38E+02 | 3.30E+02 |
| | | | | - |
| | | | | |
| $CO_2$ equi. | **2.26E+03** | 6.14E+02 | 7.99E+02 | 5.45E+02 |
| $SO_2$ equi. | **2.03E+01** | 7.51E+00 | 1.02E+01 | 7.93E+00 |

**Table 4.24 : A summary of total emissions to the impact categories for electricity options**

| Impact Categories | Global Warming Potential (GWP) kg CO2 equiv. | Human Toxicity kg 1,4-DB equiv. | Fresh Water Aqua Toxicity kg 1,4-DB equiv. | Acidification kg SO2 equiv. | Eutrophication Potential kg PO4 equiv. |
|---|---|---|---|---|---|
| | | | | | |
| EE | 2.26E+03 | 6.20E+02 | 7.86E+01 | 2.04E+01 | 3.21E+01 |
| EE-HI | 6.14E+02 | 1.13E+02 | 8.44E+00 | 7.96E+00 | 3.16E+01 |
| HE | 7.99E+02 | 1.72E+02 | 1.64E+01 | 9.82E+00 | 1.45E+01 |
| HE-HI | 5.45E+02 | 9.34E+01 | 5.52E+00 | 7.93E+00 | 1.44E+01 |

The transport options investigated the environmental performance of employing technology improvements. There are indeed environmental gains when E-FFV is compared to the E-FCV and the $H_2$-ICEV is compared to $H_2$-FCV. It is worth noting that the emissions of carbon dioxide and other major pollutants are still due to coal use in the production phase, however since for a particular bio-fuel the transport options use the same quantity of coal and hence have equivalent associated emissions, the improvement in environmental performance is due to employment of technologies with improved efficiencies. Tables 4.25 and 4.26 show that using E-FCV instead of E-FFV or H2-ICEV instead of H2-FCV has less overall emissions based on the same amount of fuel.

**Table 4.25 : A summary of coal usage (kg) and major emissions for transport options (per kilometre)**

| LCI input/output | E-FFV | E-FCV | H2-ICEV | H2-FCV |
|---|---|---|---|---|
| | kg | kg | kg | kg |
| Hard coal used for thermal requirements and coal based electricity | **1.34E+03** | **1.34E+03** | **4.38E+02** | **4.38E+02** |
| | | | | |
| | | | | |
| $CO_2$ equi. | **2.17E-01** | 1.46E-01 | 1.55E-02 | 7.97E-03 |
| $S0_2$ equi. | **1.86E-03** | 1.24E-03 | 5.57E-04 | 2.25E-04 |
| $PO_4$ equi. | **3.11E-03** | 2.09E-03 | 8.52E-04 | 4.31E-04 |

**Table 4.26 : A summary of contributions to impact categories for transport options per kilometre driven**

| Impact Categories | Warming Potential | Human Toxicity | Fresh Water Aqua Toxicity | Acidification | Eutrophication Potential |
|---|---|---|---|---|---|
| | kg CO2 equiv. | kg 1,4-DB equiv. | kg 1,4-DB equiv. | kg SO2 equiv. | kg PO4 equiv. |
| | | | | | |
| E-FFV | 2.17E-01 | 5.99E-02 | 7.70E-03 | 1.86E-03 | 3.11E-03 |
| E-FCV | 1.46E-01 | 4.03E-02 | 5.18E-03 | 1.24E-03 | 2.09E-03 |
| H2-ICEV | 1.55E-02 | 2.56E-02 | 6.61E-04 | 5.57E-04 | 8.52E-04 |
| H2-FCV | 7.97E-03 | 1.32E-02 | 3.41E-04 | 2.25E-04 | 4.31E-04 |

The previous analyses compared the individual electricity and transport options for maize energy products which addressed the secondary aims and hypotheses 2 and 3 as outlined in Chapter 3. However, the primary aim and goal of the LCA study was establish how best can maize be utilised for energy, whether it should be used to generate electrical power or used for transport purposes. Therefore Tables 4.27 and 4.28 are presented to primarily address hypothesis 1 as stated in Chapter 3.

The only way to compare the systems that result in otherwise non-comparable products (power and vehicle travel) is that of expanding the system boundaries in order to include conventional production of these system functionalities. When the systems are compared, the conventional (coal or oil-based) methods of producing electricity and transport fuel need to be added to all the scenarios to compare the scenarios on a similar energy output. Table 4.27 shows the individual additions of coal-based electricity and gasoline on a mass basis. It also shows the carbon dioxide emissions due to the employment of fossil fuels.

**Table 4.27 : A summary of fossil fuel flows and major emissions for all options after system boundary expansion**

| LCI input/output | EE | EE-HI | HE | HE-HI | E-FFV | E-FCV | H2-ICEV | H2-FCV |
|---|---|---|---|---|---|---|---|---|
| Units | kg | kg | kg | kg | kg | kg | kg | kg |
| Hard coal used for thermal requirements and coal based electricity | 1.34E+03 | 3.53E+02 | 4.38E+02 | - | 1.34E+03 | 1.34E+03 | 4.38E+02 | 4.38E+02 |
| | | | | | | | | |
| Electricity,ZA (Sys. Exp.) | 4.40E+02 | 4.40E+02 | - | - | 1.93E+03 | 1.93E+03 | 1.93E+03 | 1.93E+03 |
| Gasoline (Sys. Exp.) | 2.23E+03 | 2.23E+03 | 2.23E+03 | 2.23E+03 | 1.50E+03 | 1.13E+03 | 1.08E+03 | - |
| | | | | | | | | |
| $CO_{2\ gasoline}$ | 8.72E+03 | 8.72E+03 | 8.72E+03 | 8.72E+03 | 5.75E+03 | 4.37E+03 | 4.21E+03 | - |
| $CO_{2\ fuel\ production}$ | 1.70E+03 | 6.76E+01 | 2.53E+02 | 3.40E+00 | 1.77E+03 | 1.77E+03 | 2.55E+02 | 2.55E+02 |
| $CO_{2\ elec,\ ZA}$ | 1.11E+03 | 1.11E+03 | 4.78E+02 | 4.78E+02 | 3.29E+03 | 3.29E+03 | 3.28E+03 | 3.28E+03 |
| $CO_{2\ fossil\ (tot)}$ | 1.15E+04 | 9.90E+03 | 9.45E+03 | 9.20E+03 | 1.08E+04 | 9.44E+03 | 7.74E+03 | 3.53E+03 |
| $S0_{2\ equi.\ (fossil)}$ | 1.59E+01 | 5.74E+01 | 2.18E+01 | 6.07E+00 | 5.74E+01 | 5.66E+01 | 5.47E+01 | 5.15E+01 |
| $PO_{4\ equi.\ (fossil)}$ | 3.31E+01 | 3.23E+01 | 1.54E+01 | 2.00E+01 | 3.52E+01 | 3.50E+01 | 1.66E+01 | 1.60E+01 |

Generally, Table 4.28 shows electricity options to outscore the transport options in terms of overall major emissions for options with expanded functionality in all impact categories but global warming potential for reasons discussed in previous sections. The performance in the other impact categories is dependent on the coal emissions as discussed in previous section and the results confirm the literature findings about the polluting nature of South African coal-based electricity. The effects are strongly reduced by heat integration and Tables 4.27 and 4.28 highlight this factor for electricity options. Options that make use of the least coal are the most favourable as they present the best environmental performance. When improved vehicle technologies are compared on a broad scale with all the other options (expanded functionality) they do not present attractive environmental gains, Table 4.27 and 4.28 also highlight this aspect.

In conclusion, coal use especially for both process heating and electricity generation is highly polluting, the APR process employs less coal, and hence has a better environmental performance as displayed by hydrogen options. Heat integration options have been identified as the best option to curb coal based emissions.

**Table 4.28 : Overall emissions contributions to the impact categories for the 8 scenarios after system expansion**

| Impact Categories | Global Warming Potential (GWP) | Human Toxicity | Fresh Water Aqua Toxicity | Acidification | Eutrophication Potential |
|---|---|---|---|---|---|
| | kg CO2 equiv. | kg 1,4-DB equiv. | kg 1,4-DB equiv. | kg SO2 equiv. | kg PO4 equiv. |
| | | | | | |
| EE | **1.17E+04** | 7.44E+02 | 8.56E+01 | 3.30E+01 | 3.31E+01 |
| EE-HI | 1.01E+04 | 2.39E+02 | 1.57E+01 | 2.06E+01 | 3.25E+01 |
| HE | 9.52E+03 | 1.79E+02 | 1.63E+01 | 1.42E+01 | 1.51E+01 |
| HE-HI | 9.26E+03 | 1.01E+02 | 5.49E+00 | 1.23E+01 | 1.50E+01 |
| E-FFV | 1.13E+04 | **1.17E+03** | **1.14E+02** | **5.95E+01** | **3.52E+01** |
| E-FCV | 9.88E+03 | **1.17E+03** | **1.14E+02** | 5.86E+01 | 3.50E+01 |
| H2-ICEV | 8.18E+03 | 6.95E+02 | 4.85E+01 | 4.77E+01 | 1.62E+01 |
| H2-FCV | 3.97E+03 | 6.88E+02 | 4.85E+01 | 4.45E+01 | 1.56E+01 |

### 4.6.2 Evaluation

One of the major components of evaluation is to establish the completeness of the full required information and data for all the phases is available in an LCA. It can be concluded that there were enough data to meet the goal and scope of the study, where unavailable, assumptions were made and a sensitivity analysis carried out. A typical example is that of LCI for coal used for process heat which was essential because of unavailability of the detailed South African data. Combustion of coal was the major source of pollution, it was essential to identify whether that was dependent of the type of similar South African (categorised as hard) coal chosen. Hard coal from the EcoInvent library, one of several available libraries available in SimaPro version 7 was used. It was found that the type of hard coal chosen from different countries did not affect the results. Other issues included the use of the amount of energy needed for APR which was solely based on fundamental material balance and because no data was available for electricity requirements for APR the ethanol production electricity requirements were used.



## *4.7 Conclusions*

This chapter investigated the environmental performance of maize energy products through a life cycle assessment (LCA). First the goal and scope of the study were stated. Data were compiled and used to populate a Life Cycle Inventory (LCI), after which an LCI analysis was carried out. The individual transport and electricity options were compared through an LCIA using the impact categories that were proposed in Chapter 3. Results of system boundaries expansion in order to compare

the 8 generated options were then presented; LCIs for the expanded options were compiled and analysed. An LCIA of the expanded options was carried out and discussed. LCA interpretation discussed some of the major results and issues that emanated from the LCA study. The next chapter will briefly explore the incorporation of the APR hydrogen product into South Africa's coal-to-liquids industry for a potential of improving the environmental performance of this process and increasing its product output.

# 5 Analysis of hydrogen use in a coal to liquid refinery

## *5.1 Background*

South Africa is highly dependent on coal to meet its electricity needs, a process that has been established to be highly polluting (von Blottnitz, 2006) and with significant bearing on environmental performance of new industrial projects as shown in the previous chapters. South Africa also produces about 36% of its liquid fuel products largely from coal and a small proportion from natural gas (DME, 2006). The process of converting coal into liquid fuel products is known as Fischer-Tropsch synthesis. Both coal-based electricity generation and the coal-to-liquid process are large emitters of green house gases, in particular carbon dioxide. This chapter investigates the possibility of adding value to the coal-to-liquid process by incorporating the maize-derived hydrogen as an additional feedstock, so as to curb its carbon dioxide emissions and to produce additional synthetic fuel. Figure 5.1 illustrates this proposed concept by means of a block flow diagram. The key questions that are addressed in this chapter are: how much of the carbon dioxide emissions could be reduced and secondly how much additional synthetic fuel could be produced from a configuration presented in Figure 5.1. These two aspects will be addressed in the subsequent subsections.

## *5.2 Analysis of the proposed flowsheet*

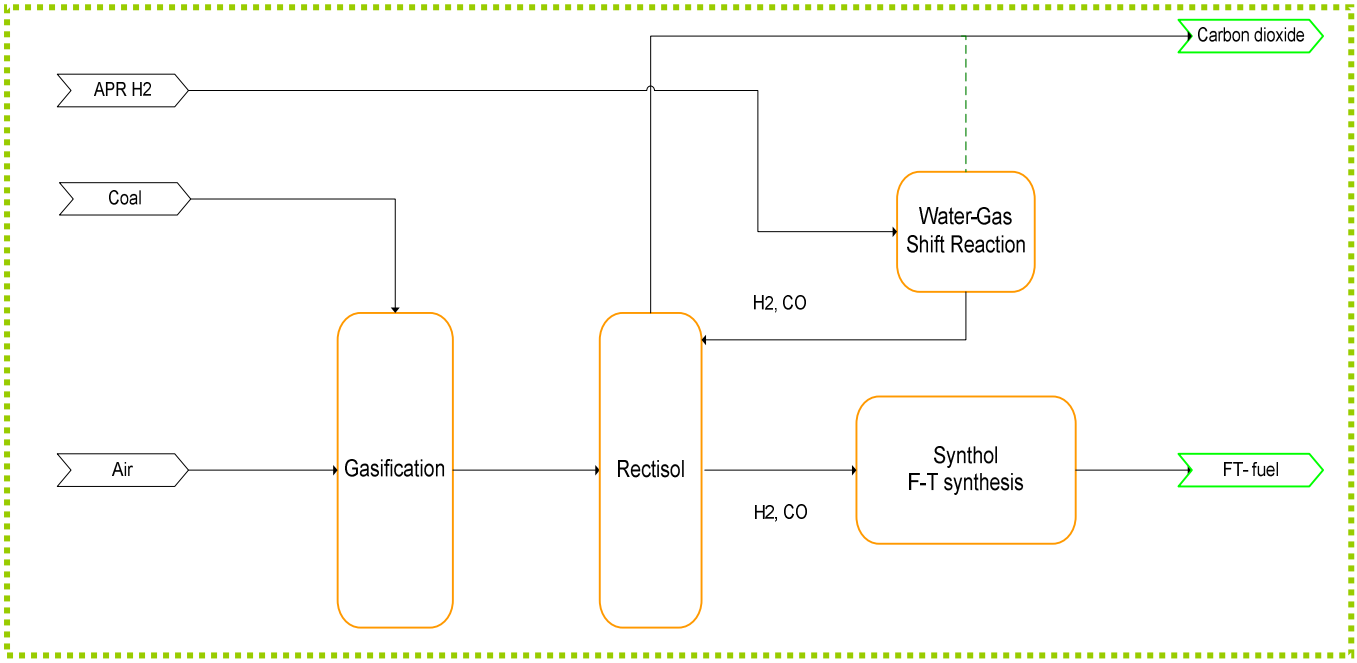


**Figure 5.1: Concept diagram for use of maize-derived hydrogen in the coal-to-liquids process**



The same reference flow employed throughout the study (viz. 3.86 tons of maize harvested from 1 hectare of land) was used for the calculations based on the configuration presented in Figure 5.1 above. It was also established in Chapter 3 that the amount of hydrogen that can be obtained from the reference flow is 348 kg.

The simplified coal to liquid process presented in Figure 5.1 is outlined briefly. Coal is fed into a vessel called a gasifier. Within the gasifier, controlled amounts of oxygen are added to break up the molecular structure of the coal. The gasifier only allows a portion of the coal to burn, resulting in the partial oxidation of the coal. This reaction produces carbon monoxide and hydrogen rich synthesis gas (or syngas) and one mole of carbon dioxide per mole of carbon monoxide. The gas that exits the gasifier is then cleaned in a unit called the Rectisol, where the syngas is stripped off the carbon dioxide which is emitted into the atmosphere; the resulting gas mixture is then fed into the Fischer-Tropsch reactor (F-T reactor). Syngas is converted to synthetic fuels over a catalyst. The process above proposes an additional unit, a water-gas shift reactor into which some of the carbon dioxide emissions are diverted and converted into carbon monoxide in the presence of APR produced hydrogen. The resulting product comprises of the syngas, water and unconverted carbon dioxide.

The water-gas shift reactor product would be sent to the Rectisol for purification, where the un-converted carbon dioxide is removed and emitted into the atmosphere. Additional synthetic fuel would be produced from the syngas produced via the water-gas shift reaction and some carbon dioxide emissions would be avoided.

Calculations were based on the two stoichiometric equations presented below, the amount of hydrogen produced from the reference flow and some assumptions:

***Water-gas shift:*** $\mathbf{CO_2 + H_2 \longleftrightarrow CO + H_2O}$

***F-T reaction:*** $\mathbf{n[2H_2 + CO] \longleftrightarrow (CH_2)n + nH_2O}$

The following assumptions were made for the analysis:

- The syngas exiting the Rectisol is in the molar proportion required for the Fischer-Tropsh synthesis reactor, viz. 2 moles of $H_2$ per mole of CO.
- For every 3 moles of $H_2$ fed into the water-gas shift reactor only 1 mole is converted, so as to attain a 2:1 molar ratio of hydrogen to carbon monoxide, essential for the F-T reactor – in other words, this reactor operates at a 33% conversion.
- All the syngas that is produced via the water-gas shift reaction is converted into gasoline, which is modelled as octane, $C_8H_{18}$.

## *5.3 Results and Discussions*

The evaluation of the results will be presented here, first the results pertaining to the amount of gasoline produced will be discussed, and subsequently the avoided carbon dioxide emissions will be discussed.

**Table 5.1: A summary of results for the proposed option**

| | | Hydrogen | Carbon dioxide | Carbon monoxide | Gasoline | Water |
|---|---|---|---|---|---|---|
| | | | | | | |
| W-G shift input | kg | 3.48E+02 | 7.65E+03 | - | - | - |
| | kmol | 1.74E+02 | 1.74E+02 | - | - | - |
| | | | | | | |
| W-G shift outlet | kg | 2.33E+02 | 5.13E+03 | 1.61E+03 | - | 1.61E+03 |
| | kmol | 1.16E+02 | 1.16E+02 | 5.74E+01 | - | 5.74E+01 |
| | | | | | | |
| F-T reactor outlet | kg | - | - | - | 8.18E+02 | 1.03E+03 |
| | kmol | - | - | - | 7.17 | 5.74E+01 |
| | l | - | - | - | 1.18E+03 | 1.03E+03 |

### 5.3.1 Additional gasoline

Table 5.1 summarises the results of the proposed scenario outlined above. These results show that for every three moles of APR hydrogen fed into the coal to liquid process, a mole of carbon dioxide is converted into an additional mole of carbon monoxide. The resulting molar ratio of hydrogen to carbon monoxide exiting as reactor product is 2:1. The unreacted carbon dioxide forms part of the water-gas shift reactor product. 348 kg (174 kmol) of hydrogen from 1 hectare of land is fed into the reactor where it is fed stoichiometrically with carbon dioxide. A third of carbon dioxide that it is fed, 57 kmol is converted as per assumptions outlined in the previous section, resulting in 57 kmol of carbon monoxide produced. Following the assumption that the resulting syngas mixture (57 kmol carbon of monoxide and 116 kmol of hydrogen) will be converted solely to gasoline as opposed to a range of possible products from an F-T reactor the amount of gasoline that results is 7.2 kmol which translates to $1.18 \times 10^3$ litre. It was important then for comparison with previous results presented in Chapter 4 to work out the additional kilometres that could be driven on the amount of gasoline produced by using hydrogen produced from maize harvested from a hectare of land. This additional distance was worked out to be to $1.18 \times 10^4$ km on an assumption that a normal vehicle driven on gasoline returns 100 km for every 10 litres used. It was deemed important to compare the number of kilometres achievable in this scenario to the ones obtained from the transport options presented in Chapter 4. The table below presents a summary of kilometres driven for all the transport options including the one produced from the coal to liquid process.

**Table 5.2: A summary of kilometres driven by the all transport options presented in the study**

| Tranport options | E-FFV | C-L ICEV | E-FCV | H2-ICEV | H2-FCV |
|---|---|---|---|---|---|
| | | | | | |
| km driven | 1.07E+04 | 1.18E+04 | 1.66E+04 | 1.59E+04 | 3.22E+04 |

It is evident from Table 5.3 that the mileage obtained from the coal-to-liquids fuelled internal combustion engine vehicle (C-L ICEV) is significantly less than that for direct use of APR hydrogen in either combustion or fuel cell engines. However it exceeds that of the ethanol flexi-fuel vehicle running on pure ethanol. The difference is not that significant amounting to about a 1000 km or 10% improvement. In weighing the two options E-FFV and C-L ICEV it is important to compare the ease of implementation in South Africa. It is worthwhile noting that in the South African context opting to produce more gasoline from the coal to liquid process as opposed to introducing ethanol fuel blends might be relatively easy and could be beneficial in short term. First, the coal to liquid industry is a well established industry; it could be assumed that expertise is available to incorporate such a process into the existing one. On the other hand several milestones would have to be reached to get to the operation of E-FFV vehicles on South African roads.

The blending of ethanol into gasoline if made mandatory in the near future still needs to be accomplished successfully first, before either importing or manufacturing Flexi-Fuel vehicles. It is evident however that those vehicles that are more efficient outperform the C-L ICEV. The GREET model (Argonne Laboratory, 2006) suggests that efficiencies of the gasoline vehicle and the E-FFV are similar, the difference in the amount of kilometres that can be delivered lies in the efficiency of the fuel production process. It turns out that the coal to liquid production process is more efficient than the ethanol production.. This can be attributed to the fact that the process utilises feedstock which would otherwise be classified as waste. Although detailed calculations were not carried out here, the thermal requirements of the water-gas shift reactor might also be met through heat integration via the bigger process's heat exchange networks due to the magnitude of the process which might be small relative the main processes, reducing its dependency on fossil based carbon dioxide emissions. On the other hand maize based ethanol is notorious for its intensive use of energy process. .

### 5.3.2 Avoided carbon dioxide emissions

The second benefit that it is realised for incorporating the APR process and water gas shift reactor into the coal to liquid process is the reduction of carbon dioxide emissions. This indicator is closely related to the replaced fossil fuels (von Blottnitz and Curran, 2007). In this instance it can be related to the amount of carbon dioxide emissions avoided from the coal to liquid process by converting them into carbon monoxide and hence the synthetic gas for the production of gasoline. The avoided carbon dioxide emissions are derived relative to the land area used to produce the biofuel that converted carbon dioxide into carbon monoxide. The amount of carbon dioxide avoided amounted to 2.52 tons per hectare of land used for biofuel production. This carbon dioxide would otherwise be emitted from Rectisol unit shown in Figure 5.1.

**Table 5.3 : Additional carbon dioxide emissions that could be obtained for operating a gasoline passenger vehicle on biofuel equivalent energy**

| | | E-FFV | H2-ICEV | E-FCV | H2-FCV | CTL-H2 |
|---|---|---|---|---|---|---|
| Maize Transport | **km** | **1.07E+04** | **1.59E+04** | **1.66E+04** | **3.22E+04** | **1.18E+04** |
| | **MJ** | 2.33E+04 | 2.47E+03 | 2.33E+04 | 2.47E+03 | 2.47E+03 |
| | **kWh** | 7.00E+02 | 7.00E+02 | 7.00E+02 | 7.00E+02 | 7.00E+02 |
| Expansion | **km added** | 2.15E+04 | 1.63E+04 | 1.55E+04 | 0.00E+00 | 3.22E+04 |
| Conversion of km added into $CO_2$ emissions | **t** | 5.74 | 4.36 | 4.15 | 0.00 | 8.60 |
| CO2 emissions from fuel prod. | **t** | 2.20 | 0.74 | 2.19 | 0.74 | 0.74 |
| Mileage on CTL | **km** | **1.18E+04** | **1.18E+04** | **1.18E+04** | **1.18E+04** | **1.18E+04** |
| tailpipe (ex CTL) | **t** | 2.70 | 2.70 | 2.70 | 2.70 | 2.70 |
| production (ex CTL) | **t** | 2.52 | 2.52 | 2.52 | 2.52 | 0.00 |
| Tot. $CO_2$ | **t** | **13.15** | **10.32** | **11.56** | **5.96** | **12.04** |
| **Total mileage** | | **4.40E+04** | **4.40E+04** | **4.40E+04** | **4.40E+04** | **4.40E+04** |

The biofuel-based transportation options replace the amount of carbon dioxide emissions that would otherwise be emitted from the use of fossil fuel they are replacing, in this case gasoline. In order to investigate CTL-$H_2$ environmental performance relative to the other transportation options, a basic system boundary expansion was carried out. When systems were expanded for the 5 transportation options, gasoline produced via the coal to liquid process was added to the previous four options, while crude based gasoline was added to the CTL-$H_2$ option and the other 3 other options to achieve the maximum mileage. The gasoline related $CO_2$ emissions for CTL-$H_2$ surpassed the worst performing transportation option (E-FFV)

by 3 tons. Although 2.52 tons of $CO_2$ emissions are avoided through the CTL-$H_2$ option, it was not enough to render a relative good performance. Table 5.1 shows that the overall emissions for CTL-$H_2$ are 12 tons closely related to 11.6 of the E-FCV, outperforming only one option (E-FFV). The hydrogen transportation options outperformed all the options.

## *5.4 Conclusions*

The aim of this Chapter was to identify conceptually the benefits of incorporating hydrogen derived from maize via an APR process into the coal to liquids process employed in South Africa. Such a use of bio-hydrogen would be aimed at adding value to the existing process by diverting some of the carbon dioxide emissions and converting it into additional synthetic fuel. Two benefits were realised based on the hydrogen produced from maize harvested from 1 hectare of land. Firstly, an additional $1.18 \times 10^3$ kg of gasoline could be produced; translating into $1.18 \times 10^4$ km driven on a normal gasoline internal combustion engine vehicle. This was found to be somewhat larger than that of the base case option of producing ethanol from maize for use in flexi-fuel vehicles. Secondly, a reduction of 2.52 tons of carbon dioxide emissions could be realised from the coal-to-liquids process, per hectare of biofuel land devoted to maize for bio-hydrogen, per year. System boundary expansion for the 5 transportations options showed the CTL-$H_2$ option only outperforming E-FFV and close in performance to E-FCV, however it was outscored by the hydrogen options.

# 6 Conclusions and Recommendations

To close off the dissertation, the key objectives of the research, as presented in Chapter 1, will now be reviewed in the light of a summary of the major findings of the research. The three hypotheses as developed in Chapters 1 and 3 will be revisited to establish how the analysis was able to support them. This chapter will first outline the motivation behind carrying out the research in Section 6.1. The objectives and major findings of the dissertation will be summarised in Section 6.2; Section 6.3 provides the validation of the hypotheses, followed by the recommendations in Section 6.4.

## *6.1 Research Motivation*

Concerns over the risks of continued fossil fuel use to sustainable development, in particular emissions of carbon dioxide, and global warming mitigation strategies have led to much research and development of alternative forms of fuel. Harnessing biomass into bio-fuels has been found to be a promising alternative; however conversion of biomass into bioenergy carriers is constrained by the low conversion efficiencies, as exemplified by the maize to ethanol route discussed in Chapters 1 and 2. New technologies that have better conversion efficiencies are constantly being developed all over the world, especially in developed countries. It is important to investigate implications of their implementation in South Africa in their developmental stage rather than adopting them in their operational stage. One such technology is the Aqueous Phase Reforming (APR) of sugar solutions into hydrogen, that could provide an alternative to fermentation into ethanol as an example of industries that APR can be transferred into. The aim of the dissertation was therefore to investigate the possible applicability of this novel United States technology in South Africa from an environmental life cycle assessment (LCA) perspective.

## *6.2 Objectives and Major Findings*

The study was aimed at addressing the following objectives:

i. To analyse the potential transfer of the APR technology into a suitable industrial sector, especially the emerging bio-fuel sector.

ii. To explore the environmental implications of employing such a technology to produce hydrogen as an energy product from agriculturally produced sugars and starches in South Africa. It was noted that it is advisable to investigate the environmental implications of such a new industrial configuration prior to suggesting any further R&D aimed at technology transfer.

The objectives were achieved by first carrying out a literature study to identify suitable industries in South Africa into which the APR process can be incorporated. Secondly, environmental benefits of eight possible industrial applications were investigated; four involving ethanol and four hydrogen, both with two vehicle options and two peak power generation options. Their environmental performances were analysed through life cycle assessment and discussed in Chapter 4, an additional industrial scenario that incorporates APR-produced hydrogen into the coal-to-liquids process was proposed and analysed in Chapter 5. The subsequent sections provide a summary of findings from literature and findings from Chapters 4 and 5.

### 6.2.1 Conclusions drawn from literature

The South African government has developed strategies and policies that address bio-fuel and hydrogen economies. The government interest in the bio-fuel industry does not only address growing environmental concerns including global warming, but envisages it also as an opportunity to contribute to the country's developmental goals, by among other issues job generation.

A second generation bio-fuel technology called the Aqueous Phase Reforming was identified to have potential in South Africa because of its higher efficiencies; however its environmental merit needed to be investigated. The sustainability of the maize to ethanol conversion route was investigated as a foundation over which the comparison with APR could be based, since they are both able to utilise the same sugar streams whilst, at the same time, this route remains environmentally controversial compared to other bio-fuel options such as sugar cane for the production of ethanol.

### 6.2.2 Environmental viability of the generated options

This subsection addresses major findings in relation to the second objective of the dissertation, resulting from work which explored the environmental implications of employing the Aqueous Phase Reforming (APR) process for harnessing 'energy

maize'. A Life Cycle Assessment (LCA) was used as an environmental sustainability tool suitable for meeting this objective. The primary goal of the study was to compare the projected environmental performance of the two maize-derived energy products, hydrogen and ethanol. Their merit was to be analysed by the impact they would have on the environment during production and when utilised to generate peak power or used as transport fuels. The following 8 generated options were defined: ethanol for generation of peak power with and without heat integration into distillery (EE and EE-HI), hydrogen for generation of peak power with and without heat integration into APR (HE and HE-HI), ethanol for use in Flexi Fuel Vehicle (E-FFV) and Fuel Cell Vehicle (E-FCV), and hydrogen use in ICE vehicle and Fuel Cell Vehicle ($H_2$-ICEV and $H_2$-FCV).

The second stage of the LCA, the development of Life Cycle Inventories (LCI) was completed as a combination of process modelling which entailed material balancing, and incorporating vehicle emission data from the GREET model. SimaPro version 7 was used for the analysis, with the EcoInvent library used to provide background life cycle inventory data.

The LCA results were evaluated based on the following impact indicators: Global Warming, Human Toxicity, Fresh Water Eco-toxicity, Acidification and Eutrophication. For comparison of the electricity and vehicle uses, it was decided that an LCA technique called system expansion as recommended by the ISO standard on LCA be used. The findings of the LCA of the 8 options is summarised below.



#### 6.2.2.1 Superiority of the APR process over the classic fermentation distillation process

The APR process for hydrogen production emerged superior over the classic fermentation-distillation process for the production of ethanol by outperforming it in all the impact categories. Process heat requirements for ethanol production were estimated to exceed those of the APR process by a factor of 10, while the electricity requirements were assumed to be similar due to lack of data for APR. All the impact categories but eutrophication (which is dependent on the amount of organic material in the effluent streams) are highly dependent on coal combustion emissions. However, the APR process emerged superior not only because of less intensive use of coal, but also because of a 40% better energy yield from the reference flow.

All analysed life cycles give off biogenic carbon dioxide, both during production of the energy product and during use, which was taken not contribute to greenhouse gas emissions hence global warming potential. For the peak power options, there are some nitrogen oxides ($NO_x$) and sulphur dioxide emissions that were evident in the emissions from the LCI analysis, these were mostly due to combustion of coal with a very small contribution from fuel combustion. The transport options also display a similar dominance of the hydrogen vehicles over the ethanol ones, also a result of better efficiencies due to less dependence on coal and higher energy yields of the hydrogen process. In all four impact categories, viz. Global Warming, Human Toxicity, Fresh-Water Eco-toxicity and Acidification, the improvement in performance of hydrogen options compared to those of ethanol ranges from 80% to 35%. The Eutrophication Potential performance is based on an assumption of half the COD concentration in the APR effluent compared to the ethanol process made in Chapter 3, which needs to be confirmed.

The dominance of the APR base options over the corresponding fermentation-distillation options remains evident after system expansion.

#### 6.2.2.2 The importance of heat integration

There are evident environmental improvements if waste heat from peak power generation could be re-incorporated into the APR process and the distillery for the ethanol production. Preliminary calculations showed a coal use reduction of 90% for the ethanol distillery and a total replacement for APR thermal process energy needs, with the potential for heat exports (which was however not included in further assessment). The performance of the 4 impact categories that depend on coal emissions were reduced by similar factors, indicating the extent of coal emissions contribution in the bio-fuels production phase as opposed to their end-use. The Eutrophication still displays similar results for options with or without heat integration for reasons stipulated in Section 6.2.2.1 above.

#### 6.2.2.3 Superiority of fuel cells vehicles over internal combustion engines vehicles

It is well known that fuel cell vehicles are more efficient than their internal combustion engine vehicle counterparts. More mileage was obtained for a fuel cell vehicle operating on a set amount of bio-fuel derived from the LCA reference flow. The hydrogen fuel cell vehicle emerged the most efficient of the four transport fuel

use options studied, and hence displayed the best environmental performance. The results from the GREET model (Argonne Laboratory, 2006) showed the ethanol flexi fuel vehicle to have a similar efficiency to that of a gasoline internal combustion engine vehicle, while the E-FCV vehicle is about 48% more efficient than the E-FFV, a result that translated to better environmental performance by a similar factor. The $H_2$-ICEV is 20% more efficient than the gasoline vehicle, while the $H_2$-FCV is predicted to be highly superior with efficiency gains of more than 130%. This section can be summed up as follows: the more efficient the vehicle, the better the environmental performance of the field-to-wheel system in which it is used.

#### 6.2.2.4 Evaluation of the use of ethanol or hydrogen for peak power as opposed to transport fuels

For comparison of the peak power generation options and the vehicle options, system expansion as recommended by the ISO standard on LCA was carried out. The results generally showed a superiority of the electricity options over the vehicle options. The electricity options outperformed the vehicle options in all the impact categories but global warming potential, where the difference was small with exception of outstanding performance of the $H_2$ FCV. This was attributed to the addition of coal based electricity to vehicle options to render the systems equal. This was despite the corresponding addition of large mileages of gasoline-propelled vehicles into the electricity options, due to a high efficiency of the hydrogen fuel cell vehicle.

It could be argued that, since the energy products were used for peak power, it was inappropriate to use coal-base load in the system expansion instead of using other options such as pump storage on the back of the coal base load or new open cycle turbines running on diesel. The former option would further exaggerate the dirtiness of coal due to the efficiency losses; however both options could be a subject for further study.

It was established through literature and verified in this study that South African coal-based electricity is highly polluting, more polluting than gasoline refining and fuel combustion in vehicles, which have better pollution reduction measures installed to reduce the amount of pollutants that are emitted into the atmosphere. Gasoline from crude oil was used for system expansion, an assumption that was not justified by any analysis of which type of gasoline (crude-derived or CTL synthetic) is more

likely to be displaced by biofuels in South Africa. It should be noted that coal-based gasoline is more polluting, but also that data for its production is not available in an LCA format, an aspect that can be explored in a future project.

It was identified that the control of toxic pollutants such as sulphur oxides and nitrogen oxides during gasoline production and use do not translate to reduced carbon dioxide emissions hence, the poorer environmental performance of the electricity options in the global warming category.

The transportation options generally showed a worse performance, it was therefore decided to explore another transportation option that might have better environmental gains.

#### 6.2.2.5 An analysis of incorporating APR in the coal to liquid process

Based on the study motivation presented above, it was proposed that the APR process be incorporated into the coal-to-liquids process to reduce the amount carbon dioxide emissions. An additional unit, the water-gas shift reactor was proposed to convert some of carbon dioxide emissions using the APR-produced hydrogen into carbon monoxide and ultimately into more synthetic gas (syngas). The syngas would then be converted into additional synthetic fuel in the Fischer Tropsch process. The additional synthetic fuel produced was calculated based on the LCA reference flow, maize harvested from 1 hectare of land (3.86 tons). A total of 2.5 tons of carbon dioxide emissions could be avoided, and gasoline product yield improved to result in an additional 11 800 vehicle kilometres, which exceeds the 10 700 km of the E-FFV option by about 10 %. When basic system expansion was carried out for the 5 transportation options, CTL-$H_2$ only outscored E-FFV while having a close performance to E-FCV. The hydrogen options still emerged superior.

## *6.3 Validation of hypotheses*

As indicated in Chapters 1 and 3 the thesis aimed to test the following hypotheses:

1. Using energy products derived from maize for electricity generation as opposed to vehicle fuel is environmentally attractive in South Africa because of the relatively high environmental impact of the coal-based electricity.

System expansion in a life cycle analysis of the energy utilisation options as suggested by the ISO were carried out to test this hypothesis. The electricity options for both ethanol and hydrogen outscored their vehicle options counterparts in four of the impact categories, performing poorer only in global warming potential impact. This was due to the polluting nature of coal-based electricity. The idea that there are better environmental gains when the "dirtiest" fuel is replaced by a cleaner burning one was confirmed.

2. Where electricity is to be generated from the maize-derived energy products, heat integration into the production plant by means of combined heat and power (CHP) has better energy yields and environmental benefits compared to electricity generation without heat integration.

The amount of coal required for process heat for ethanol production would be reduced by 90%, while it would eliminated altogether for the production of hydrogen after heat integration. This would translate into improved net energy yields due to reduced dependence on coal. Coal was established as the biggest polluter throughout the study, thus its reduction resulted in highly improved environmental performance in all the impact categories studied.

3. The environmental performance of both the ethanol and the hydrogen options can be improved not only by changes in production efficiency, but also by technology improvements in the product use-phase.

When ethanol and hydrogen were utilised as transport fuels, two types of vehicles were opted for, the internal combustion engine vehicles and the more technologically improved fuel cell vehicles. An improvement in the efficiency

would be evident from an improved mileage from the same amount of fuel. The efficiency improvement would translate to better environmental performances in all the impact categories in their LCA analysis.

## *6.4 Recommendations*

The following recommendations can now be made based on the conclusions drawn from the analysis presented in the research:

### 6.4.1 Short-to-medium term options

With production of ethanol already in the pipeline in South Africa, it is recommended that ethanol be utilised for peak power generation as opposed to transport fuel as a short term option, as it presents a more environmentally attractive option. APR produced hydrogen is also best utilised for electricity generation, this presents a medium-term option, since it might take years still before for the hydrogen vehicle market is well established in South Africa.

Although preliminary results showed an improved environmental performance after heat integration through CHP into the distillery and APR process for peak power generation options due to reduced coal dependence, it is recommended that further work be carried out on the viability and efficiency of heat integration.

On the other hand, the incorporation of the APR process into the coal-to-liquids process also presents another medium term option; although this option outperforms the ethanol flexi fuel vehicle (E-FFV) by only 10% its implementation could be relatively easy.

### 6.4.2 Long term options

Long term options include the use of the energy products in fuel cell vehicles which present better environmental gains than the internal combustion engine vehicle. $H_2$-FCV presents the most environmentally attractive long term option especially if coal-based electricity is replaced by other renewables. However, it might still take a few years for these vehicles to be well established in the market.

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# Appendices

# Appendix A1: Background and major assumptions

## Introduction to LCA

The worksheet contains a summary of preliminary mass and energy balance for LCI (life cycle inventory) for the LCA.

The Life Cycle Assessment is aimed at comparing the environmental performances of the corn to (ethanol and hydrogen) energy products.

The reference flow for the systems under consideration is maize produced from 1 hectare of land.

All the processes prior to sacchirification are not included in the LCA as they are similar

### General statistics and assumptions

| Corn production in South Africa | | | | |
|---|---|---|---|---|
| | | | | |
| 2005/2006 | | | www.grainsa.co.za | |
| | | | | |
| | | | | |
| | Planted Land | | 1.55E+06 | Hec. |
| | | | | |
| | Maize Prod. | | 5.99E+06 | Tons |
| | | | | |
| | Yield | | 3.86 | tons/hec. |
| | | | 3859.30 | kg/hec |

**Starch Content in Maize** www.fao.org http://www.sagl.co.za/maize_analysis.aspx

| | | | | |
|---|---|---|---|---|
| | Percentage | | | 70% |
| | | | | |
| Other components in maize | | | | 30% |

**2005/06 statistics**

**Percentage of corn converted to glucose** www.lsbu.co.uk, www.fao.org/docrep, (Wilson et al., 2004)

99%

### Mass Balance Basis

| Glucose from corn | | 2674.49 | kg |
|---|---|---|---|
| | | 2.67 | tonnes |
| | | | |
| Spent grain | | 1.16E+03 | kg |

## Energy yields of maize ethanol and hydrogen:

| | | |
|---|---|---|
| LHV for maize cobs | **15.2** | **MJ/kg** |
| Maize yield | **3.86** | **kg/hectare** |
| Energy available from maize | **5.87E+04** | **MJ/hectare** |
| Energy from maize per basis | **5.87E+04** | **MJ** |
| | | |
| Ethanol produced | **1.29E+03** | **kg** |
| LHV for ethanol | **25.1** | **MJ/kg** |
| | | |
| Gross energy from ethanol | **3.24E+04** | **MJ** |
| | | |
| **Gross from ethanol/Gross energy from maize cobs** | **55%** | |
| | | |
| Hydrogen produced | **348** | **kg/hectare** |
| LHV for hydrogen | **120.1** | **MJ/kg** |
| | | |
| Gross energy from hydrogen | **4.18E+04** | **MJ** |
| | | |
| **Gross from hydrogen/Gross energy from maize cobs** | **71%** | |

# Appendix A2: Material Balance

## Mass and energy balance over the corn to ethanol flowsheet

### Physical properties and general information

**Relevant reactions (Fermentation reaction)**

$C_6H_{12}O_6$ ====> $2(CH_3CH_2OH)$ + $2(CO_2)$
Sugar ====> Alcohol + Carbon dioxide gas
(Glucose) (Ethyl alcohol)

| **Reaction assumptions** | (Ljiljana et. al, 2006 & Krishnan et. al., 2000) | |
|---|---|---|
| Concentration of sugars in a fermentor | 17.5 | wt.% |
| Conversion of glucose into ethanol | 98% | wt. |
| Recovery ratio of ethanol from distillatio | 0.96 | |

| **Molar mass of compounds** | Perry (Section 2) | |
|---|---|---|
| **Compounds** | **Mol. Mass** | |
| Glucose | 180 | kg/kmol |
| Ethanol | 46 | kg/kmol |
| Carbon dioxide | 44 | kg/kmol |
| Water | 18 | kg/kmol |

| **Physical Properties** | | |
|---|---|---|
| Ethanol | Bernesson Sven et. al, (2006) | |
| Density of water | 1000 | $kg/m^3$ |
| Density of ethanol | 789 | $kg/m^3$ |
| Energy density | 25.1 | MJ/kg (LLV) |

| **Energy requirements for ethanol production** | (Kim & Dale et. al., 2005) | |
|---|---|---|
| Total | 17 | MJ/kg |
| Thermal | 14.5 | MJ/kg |
| Electricity | 2.6 | MJ/kg |

| **Energy usage of sub-section in dry milling** | Kim and Dale, 2005 | |
|---|---|---|
| **Sub-process** | **% fraction** | |
| Milling | 0.8% | |
| Liquefaction/saccharification | 29.7% | Outside the system boundaries |
| Fermentation | 3.5% | |
| Distllation | 56.5% | |
| DDG's recovery | 9.6% | |

| **Unit conversions** | | |
|---|---|---|
| 1 gallon | 3.79 | litres |
| 1 acre | 0.41 | hectares |
| 1 MJ | 0.28 | kWh |
| 1 Btu | 1055 | Joules |

## Heat Capacity

$Cp = CPVAPA + (CPVAPB)*T + (CPVAPC)*T^2$

| | | | |
|---|---|---|---|
| Ethanol | 9.014 | 2.14E-01 | -8.39E-05 |
| Water | 32.243 | 1.94E-03 | 1.06E-05 |
| Carbon monoxide | 30.869 | -1.29E-02 | 2.79E-05 |
| Carbon dioxide | 19.795 | 7.34E-02 | -5.60E-05 |

| | | |
|---|---|---|
| Cp of liquid ethanol | 1.12E+02 | J/mol K |
| Cp of liquid water | 7.53E+01 | J/mol K |

| Streams | Ferm. In. | Ferm Out | $CO_2$ Out | In Distillation | Ethanol product | Dist. Bottoms (stillage) |
|---|---|---|---|---|---|---|
| **Molar Flow (kmol)** | **7.20E+02** | **7.63E+02** | **2.91E+01** | **7.34E+02** | **3.17E+01** | **7.02E+02** |
| **Mass Flow (kg)** | **1.54E+04** | **1.54E+04** | **1.28E+03** | **1.41E+04** | **1.35E+03** | **1.39E+04** |
| **Volume (ethanol) $m^3$** | | | | | **1.63E+00** | |
| **Volume $m^3$** | | | | | **1.70E+00** | |
| | | | | | | |
| **Mass Flow (kg)** | | | | | | |
| Glucose | 2.67E+03 | 5.35E+01 | - | 5.35E+01 | - | 5.35E+01 |
| Water | 1.27E+04 | 1.27E+04 | - | 1.27E+04 | 6.79E+01 | 1.26E+04 |
| Carbon dioxide | - | 1.28E+03 | 1.28E+03 | - | - | - |
| Ethanol | - | 1.34E+03 | - | 1.34E+03 | 1.29E+03 | 5.36E+01 |
| spent grains | 1.16E+03 | 1.16E+03 | - | 1.16E+03 | | 1.16E+03 |
| | | | | | | |
| **Mol Flow (kmol)** | | | | | | |
| Glucose | 1.49E+01 | 2.97E-01 | - | 2.97E-01 | - | 2.97E-01 |
| Water | 7.05E+02 | 7.05E+02 | - | 7.05E+02 | 3.77E+00 | 7.01E+02 |
| Carbon dioxide | - | 2.91E+01 | 2.91E+01 | - | - | - |
| Ethanol | - | 2.91E+01 | - | 2.91E+01 | 2.80E+01 | 1.16E+00 |

## Energy calculations

Overall energy requirements

| | |
|---|---|
| **Thermal** | **1.86E+04MJ** |
| **Electricity** | **9.29E+02kWh** |

Coal for process heat is based on an assumption on coal boilers efficiency of **80%**

Energy (thermal) requirements for ethanol fermentation and distillation

| | |
|---|---|
| **Fermentation** | **8.16E+02MJ** |
| **Distillation** | **1.32E+04MJ** |

Electricity requirements for ethanol fermentation and distillation

| | |
|---|---|
| **Fermentation** | **40.6kWh** |
| **Distillation** | **656.0kWh** |

| | |
|---|---|
| Caloric value of coal | **23MJ/kg** |
| Amount of electricity that can be deduced from coal | **2.11kWh/kg** |
| Coal used for thermal heating | **1.01E+03kg** |
| Amount of coal required | **1.34E+03kg** |

**Net energy calculations**

| | |
|---|---|
| Total energy inherent in the ethanol (Gross energy) | **3.23E+04MJ** |

| Streams | In APR (react.) | Reforming | W-G Shift | Hydrogen Prod. | Liquid phase | Hydrogen stream | $CO_2$ Stream |
|---|---|---|---|---|---|---|---|
| **Molar Flow (kmol)** | 7.20E+02 | 8.80E+02 | 8.80E+02 | 2.61E+02 | 6.19E+02 | 1.75E+02 | 8.65E+01 |
| **Mass Flow (kg)** | 1.54E+04 | 1.54E+04 | 1.54E+04 | 3.48E+02 | 1.23E+04 | 3.72E+02 | 3.81E+03 |
| **Volume m^3/hect** | | | | | | | |
| **Mass Flow (kg)** | | | | | | | |
| Glucose | 2.67E+03 | 5.35E+01 | 5.35E+01 | | 5.35E+01 | | |
| Water | 1.27E+04 | 1.27E+04 | 1.11E+04 | | 1.11E+04 | | |
| Carbon dioxide | - | - | 3.81E+03 | | - | | 3.81E+03 |
| Carbon monoxide | - | 2.45E+03 | 2.45E+01 | | - | 2.45E+01 | |
| Hydrogen | - | 1.75E+02 | 3.48E+02 | 3.48E+02 | - | 3.48E+02 | |
| Other products(alkanes) | | | | | | | |
| Spent grain | 1.16E+03 | 1.16E+03 | 1.16E+03 | - | 1.16E+03 | | |
| **Mol Flow (kmol)** | | | | | | | |
| Glucose | 1.49E+01 | 2.97E-01 | 2.97E-01 | - | 2.97E-01 | | - |
| Water | 7.05E+02 | 7.05E+02 | 6.18E+02 | - | 6.18E+02 | | - |
| Carbon dioxide | - | - | 8.65E+01 | 8.65E+01 | - | - | 8.65E+01 |
| Carbon monoxide | - | 8.74E+01 | 8.74E-01 | 8.74E-01 | - | 8.74E-01 | - |
| Hydrogen | - | 8.74E+01 | 1.74E+02 | 1.74E+02 | - | 1.74E+02 | - |

| | | | |
|---|---|---|---|
| **Energy required from coal** | **2.47E+03** | **MJ** | |
| **Amount of coal based electricity** | **6.97E+02** | **kWh** | |
| **Total coal needed** | **4.38E+02** | **kg** | |

| | Hin APR kJ | | Hout APR kJ | |
|---|---|---|---|---|
| **Glucose** | 3.98E+03 | | 1.63E+04 | |
| **Hydrogen** | - | | 6.51E+05 | |
| **Water** | 5.33E+06 | | 5.62E+06 | |
| **Carbon monoxide** | - | | 5.42E+03 | |
| **Carbon dioxide** | - | | 4.51E+05 | |
| | | | | |
| **Total Enthalpy** | **5.33E+06** | | **6.74E+06** | |
| | | | | |
| | | | | |
| **Reactor heat requirements** | | | **1.98E+03** | **MJ** |

| | | | |
|---|---|---|---|
| **Energy required from coal** | **2.47E+03** | **MJ** | |
| **Amount of coal based electricity** | **6.97E+02** | **kWh** | |
| **Total coal needed** | **4.38E+02** | **kg** | |

# Appendix A3: Electricity options

## Ethanol Electricity

| Net energy calculations | |
|---|---|
| Total energy inherent in the ethanol (Gross energy) | **3.23E+04** MJ |
| **Energy produced from a 35% efficient engine** | **1.13E+04 MJ** |

## Associated emissions

| $CO_2$ | $NO_x$ | CO | $PM_{10}$ | Strachan and Farrel, 2006 |
|---|---|---|---|---|
| **g/kWh** | **g/kWh** | **g/kWh** | **g/kWh** | |
| 300 | 0.29 | 0.42 | 0.041 | |
| **kg** | **kg** | **kg** | **kg** | |
| 2.69E+03 | 2.60E+00 | 3.77E+00 | 3.68E-01 | |

## CHP calculations for electricity options

**Stillage composition**

| BOD | COD | Nitrogen (tot.) | Phos.(total) | Sulphur (tot) |
|---|---|---|---|---|
| **g/L** | **g/L** | **mg/L** | **mg/L** | **mg/L** |
| 12.93 | 17.82 | 163.8 | 68.4 | 89.7 |
| **kg** | **kg** | **kg** | **kg** | **kg** |
| 179.49 | 247.37 | 2.27 | 0.95 | 1.25 |

**Conversion of stillage to energy**

Methane production from corn thin stillage

For a thin stillage of **1 kg COD** Methane production: **0.342 $m^3$ methane**

Methane percentage in the biogas **80%**

Caloric value of methane is **39 $MJ/m^3$** **LHV**

Boiler efficiency for the production of steam from biogas **85%**

The amount of COD in thin stillage

**247.37 kg COD** **84.60** $m^3$ methane rich gas is produced from the COD

Energy that can be produced from the stillage **2.24E+03 MJ**

**Heat calculation in a gas turbine CHP setup (from gas exhaust)**

| | |
|---|---|
| For Gas turbine use only, electicity production efficiency of the process is | **35%** |
| For CHP, heat is produced together with electricity with a total CHP efficiency of | **80%** |
| Power to heat ratio is between 0.4-0.7, taking the intermidiate value of | **55%** |

**Power/Heat Ratio = CHP electricity output (MJ)/ Useful heat output**

| | |
|---|---|
| CHP electricity output | **1.13E+04 MJ** |
| Useful heat output | **2.05E+04 MJ** |
| Additional process heat for the production process | |
| **CHP, useful heat output** | **2.05E+04 MJ** |
| **Energy generated from anaerobic digestion of stillage** | **2.24E+03 MJ** |
| Total heat generated from gas turbine exhaust and biogas from stillage | **2.28E+04 MJ** |
| Energy needed from coal after heat integration (gas exhaust and AE of stillage) | **5.24E+02 MJ** |
| Amount of coal required | **22.8 kg** |

**Emissions from LCI analysis in SimaPro**

| | | | EtoH elec. | EtoH elec. Heat Integration |
|---|---|---|---|---|
| Carbon dioxide, biogenic | Air | g | 347.10 | 346.99 |
| Carbon dioxide, fossil | Air | g | 186.00 | 49.70 |
| Carbon monoxide, fossil | Air | mg | 176.00 | 16.60 |
| Methane, fossil | Air | mg | 599.61 | 211.00 |
| Nitrogen oxides | Air | mg | 735.00 | 393.00 |
| Particulates, < 10 um | Air | mg | 12.70 | 17.60 |
| Sulfur dioxide | Air | g | 1.20 | 0.42 |
| COD, Chemical Oxygen Demand | Water | g | 73.03 | 73.01 |
| BOD5, Biological Oxygen Demand | Water | g | 59.20 | 52.92 |
| Nitrate | Water | µg | 231.00 | 50.40 |

## Hydrogen Electricity

| | |
|---|---|
| Energy inherent in hydrogen | **4.18E+04 MJ**<br>**1.16E+04 kWh** |
| For electricity production assume overall efficiency of | **35%** |
| Electricity produced | **1.46E+04 MJ**<br>**4.06E+03 kWh** |

**Emissions to air**

| | | | |
|---|---|---|---|
| **$NO_x$** | **g/kWh** | **0.29** | **g** |
| | | **3.36** | **kg** |

**Stillage composition**

| BOD | COD | Nitrogen (tot. | Phos.(total) | Sulphur (tot) |
|---|---|---|---|---|
| g/L | g/L | mg/L | mg/L | mg/L |
| 6.48 | 8.91 | 81.9 | 34.2 | 44.85 |
| | | | | |
| kg | kg | kg | kg | kg |
| 79.96 | 109.94 | 1.01 | 0.42 | 0.55 |

**Conversion of stillage to energy**

Methane production from corn thin stillage

| For a thin stillage of | | Methane production | |
|---|---|---|---|
| **1 kg COD** | | **0.342** | $m^3$ methane |
| Methane percentage in the biogas | | **80%** | |
| Caloric value of methane is | | **39** | **MJ/$m^3$** **LHV** |
| Boiler efficiency for the production of steam from biogas | | **85%** | |
| The amount of COD in thin stillage | | | |
| **109.94 kg COD** | | **37.60** | $m^3$ methane rich gas is produced from the COD |
| Energy from the stillage | | **9.97E+02** | **MJ** |

**Utilising gas turbine exhaust to generate additional process heat**

| | |
|---|---|
| For Gas turbine use only, electicity production efficiency of the process is | 35% |
| For CHP, heat is produced together with electricity with an total CHP efficien | 80% |
| Power to heat ratio is between 0.4-0.7, taking the intermidiate value of | 55% |

**Power/Heat Ratio = CHP electricity output (MJ)/ Useful heat output**

| | | |
|---|---|---|
| CHP electricity output | **1.46E+04** | **MJ** |
| Useful heat output | **2.66E+04** | **MJ** |

**Total useful heat generated to provide process heat**

| | | |
|---|---|---|
| CHP, useful heat output | **2.66E+04** | **MJ** |
| Energy generated from anaerobic digestion of stillage | **9.97E+02** | **MJ** |
| Total heat generated | **2.76E+04** | **MJ** |
| Energy from coal essential for prod. of hydrogen | **-4.57E+03** | **MJ** |
| | **-1.27E+03** | **kWh** |
| Potential energy export | **-3.21E+04** | **MJ** |
| | **-1.40E+03** | **kg** |

**Emissions from LCI analysis in SimaPro**

| | | | H2 elec. | H2 elec. Heat Integration |
|---|---|---|---|---|
| Carbon dioxide, biogenic | Air | g | 266.78 | 266.77 |
| Carbon dioxide, fossil | Air | g | 50.20 | 33.90 |
| Carbon monoxide, fossil | Air | mg | 18.66 | 7.86 |
| Methane, fossil | Air | mg | 26.50 | 151.00 |
| Nitrogen oxides | Air | mg | 408.00 | 367.00 |
| Particulates, < 10 um | Air | mg | 9.79 | 9.79 |
| Sulfur dioxide | Air | mg | 0.38 | 0.30 |
| COD, Chemical Oxygen Demand | Water | g | 24.85 | 24.85 |
| BOD5, Biological Oxygen Demand | Water | g | 18.10 | 18.10 |
| Nitrate | Water | µg | 54.70 | 33.10 |

## Impact category results for the electricity options

| Impact categories | EE | HE | EE-HI | HE-HI |
|---|---|---|---|---|
| global warming (GWP100) | 2.00E-01 | 5.47E-02 | 5.44E-02 | 3.73E-02 |
| human toxicity | 5.49E-02 | 1.18E-02 | 1.00E-02 | 6.39E-03 |
| acidification | 6.96E-03 | 1.12E-03 | 7.47E-04 | 3.77E-04 |
| fresh water aquatic ecotox. | 1.81E-03 | 6.72E-04 | 7.04E-04 | 5.43E-04 |
| eutrophication | 2.85E-03 | 9.90E-04 | 2.80E-03 | 9.84E-04 |

# Appendix A4: Transport options

| | | | | | |
|---|---|---|---|---|---|
| **Energy produced from ethanol** | | | | **3.23E+04** | **MJ** |
| **Energy produced from hydrogen** | | | | **4.18E+04** | **MJ** |
| | **$H_2$ SI vehicle** | **$H_2$ Fuel Cell Vehicle** | **EtOH FFV** | **EtOH FCV** | |
| **Gasoline equiv. MPG** | **1.2** | **2.32** | **1.0** | **1.48** | **Greet 1.7** |
| **Distance travelled (km)** | **1.66E+04** | **3.22E+04** | **1.07E+04** | **1.59E+04** | |

**Greet Model, 2007**

**Gasoline Vehicle: CG and RFG/ emissions (g/mile)**

| Item | Fuel production | Electrical Scenarios | E-FFV | $H_2$-ICEV | E-FCV | $H_2$- FCV |
|---|---|---|---|---|---|---|
| | g/mile | kg | kg | kg | kg | kg |
| CO2 | 72 | 1.45E+03 | 9.65E+02 | 6.99E+02 | 7.34E+02 | 0.00E+00 |
| CH4 | 0.083 | 1.67E+00 | 1.11E+00 | 8.06E-01 | 8.46E-01 | 0.00E+00 |
| N2O | 0.006 | 1.22E-01 | 8.14E-02 | 5.89E-02 | 6.19E-02 | 0.00E+00 |
| GHGs | 76 | 1.52E+03 | 1.01E+03 | 7.35E+02 | 7.71E+02 | 0.00E+00 |
| VOC: Total | 0.109 | 2.20E+00 | 1.47E+00 | 1.06E+00 | 1.12E+00 | 0.00E+00 |
| CO: Total | 0.039 | 7.76E-01 | 5.18E-01 | 3.75E-01 | 3.94E-01 | 0.00E+00 |
| NOx: Total | 0.114 | 2.30E+00 | 1.54E+00 | 1.11E+00 | 1.17E+00 | 0.00E+00 |
| PM10: Total | 0.051 | 1.03E+00 | 6.90E-01 | 4.99E-01 | 5.24E-01 | 0.00E+00 |
| PM2.5: Total | 0.018 | 3.71E-01 | 2.48E-01 | 1.79E-01 | 1.88E-01 | 0.00E+00 |
| SOx: Total | 0.063 | 1.27E+00 | 8.49E-01 | 6.15E-01 | 6.46E-01 | 0.00E+00 |
| VOC: Urban | 0.069 | 1.39E+00 | 9.30E-01 | 6.73E-01 | 7.07E-01 | 0.00E+00 |
| CO: Urban | 0.018 | 3.62E-01 | 2.41E-01 | 1.75E-01 | 1.83E-01 | 0.00E+00 |
| NOx: Urban | 0.048 | 9.65E-01 | 6.43E-01 | 4.66E-01 | 4.89E-01 | 0.00E+00 |
| PM10: Urban | 0.009 | 1.90E-01 | 1.27E-01 | 9.18E-02 | 9.64E-02 | 0.00E+00 |
| PM2.5: Urban | 0.005 | 1.10E-01 | 7.35E-02 | 5.32E-02 | 5.59E-02 | 0.00E+00 |
| SOx: Urban | 0.030 | 6.10E-01 | 4.07E-01 | 2.94E-01 | 3.09E-01 | 0.00E+00 |

| Item | Electrical Scenarios | E-FFV | $H_2$-ICEV | E-FCV | $H_2$- FCV |
|---|---|---|---|---|---|
| | kg | kg | kg | kg | kg |
| CO2 | 8.60E+03 | 5.74E+03 | 4.15E+03 | 4.36E+03 | 0.00E+00 |
| CH4 | 1.96E+00 | 1.31E+00 | 9.48E-01 | 9.95E-01 | 0.00E+00 |
| N2O | 3.63E-01 | 2.42E-01 | 1.75E-01 | 1.84E-01 | 0.00E+00 |
| GHGs | 8.75E+03 | 5.84E+03 | 4.23E+03 | 4.44E+03 | 0.00E+00 |
| VOC: Total | 5.82E+00 | 3.88E+00 | 2.81E+00 | 2.95E+00 | 0.00E+00 |
| CO: Total | 7.61E+01 | 5.08E+01 | 3.67E+01 | 3.86E+01 | 0.00E+00 |
| NOx: Total | 5.14E+00 | 3.43E+00 | 2.48E+00 | 2.61E+00 | 0.00E+00 |
| PM10: Total | 1.61E+00 | 1.07E+00 | 7.77E-01 | 8.16E-01 | 0.00E+00 |
| PM2.5: Total | 6.69E-01 | 4.46E-01 | 3.23E-01 | 3.39E-01 | 0.00E+00 |
| SOx: Total | 1.39E+00 | 9.27E-01 | 6.71E-01 | 7.05E-01 | 0.00E+00 |
| VOC: Urban | 3.65E+00 | 2.43E+00 | 1.76E+00 | 1.85E+00 | 0.00E+00 |
| CO: Urban | 4.72E+01 | 3.15E+01 | 2.28E+01 | 2.39E+01 | 0.00E+00 |
| NOx: Urban | 2.73E+00 | 1.82E+00 | 1.32E+00 | 1.38E+00 | 0.00E+00 |
| PM10: Urban | 5.48E-01 | 3.65E-01 | 2.65E-01 | 2.78E-01 | 0.00E+00 |
| PM2.5: Urban | 2.95E-01 | 1.97E-01 | 1.43E-01 | 1.50E-01 | 0.00E+00 |
| SOx: Urban | 6.82E-01 | 4.55E-01 | 3.29E-01 | 3.46E-01 | 0.00E+00 |

## Results from LCI analysis in SimaPro

| | | | E-FFV | H2-ICEV | E-FCV | H2-ICEV |
|---|---|---|---|---|---|---|
| Carbon dioxide, biogenic | Air | g | 371.17 | 234.35 | 250.53 | 120.81 |
| Carbon dioxide, fossil | Air | g | 205.00 | 44.30 | 138.00 | 23.00 |
| Carbon monoxide, fossil | Air | mg | 190.00 | 23.50 | 127.50 | 12.00 |
| Carbon monoxide, biogenic | Air | g | 2.50 | 0.81 | 1.20 | 0.00 |
| Methane, fossil | Air | mg | 659.74 | 175.00 | 443.98 | 90.10 |
| Nitrogen oxides | Air | mg | 533.94 | 350.00 | 435.00 | 149.00 |
| Particulates, < 10 um | Air | mg | 33.00 | 29.20 | 29.80 | 24.90 |
| Sulfur dioxide | Air | g | 1.29 | 0.35 | 0.87 | 0.18 |
| COD, Chemical Oxygen Demand | Water | g | 80.36 | 22.05 | 54.08 | 11.37 |
| BOD5, Biological Oxygen Demand | Water | g | 58.25 | 16.09 | 39.20 | 8.29 |
| Nitrate | Water | mg | 1.88 | 0.02 | 1.27 | 0.01 |

## LCIA results from SimaPro

| Impact categories | E-FFV | E-FCV | H2-ICEV | H2-FCV |
|---|---|---|---|---|
| global warming (GWP100) | 2.20E-01 | 1.48E-01 | 4.85E-02 | 2.50E-02 |
| human toxicity | 6.03E-02 | 4.05E-02 | 1.04E-02 | 5.27E-03 |
| acidification | 7.66E-03 | 5.15E-03 | 9.94E-04 | 5.13E-04 |
| fresh water aquatic ecotox. | 1.89E-03 | 1.26E-03 | 5.57E-04 | 2.55E-04 |
| eutrophication | 3.11E-03 | 2.09E-03 | 8.68E-04 | 4.39E-04 |

# Appendix A5: System expansion

## Assumptions for the production for coal electricity

| | | | | |
|---|---|---|---|---|
| Unit conversion | 1 kWh | 3.6 | MJ | |
| Caloric value of coal | | 23 | MJ/kg | |
| | | 6.39 | kWh/kg | |
| **Molar mass of CO2** | | 44 | kg/kmol | |
| **Molar mass of C** | | 12 | kg/kmol | |
| | | | | |
| Assuming the overall efficiency from electricity from coa | | 33% | | |
| Therefore electricity from coal | | 2.11 | kWh/kg | |
| CO2 released from 1kg of coal | | 1.8 | kg/kg coal | Eskom |
| Carbon produced | | 0.49 | kg/kg coal | |

## Assumptions for associated with gasoline

| | | | |
|---|---|---|---|
| Energy density of octane (gasoline) | 30.1 | MJ/l | LHV |
| | 43.50 | MJ/kg | |
| Density of octane | 0.692 | kg/l | |
| Density of ethanol | 0.789 | kg/l | |
| Energy density of ethanol | 21.1 | MJ/l | |
| | 26.7 | MJ/kg | |
| Percentage of C in gasoline | 85% | Calculated | |
| Ethanol produced from corn | 1286.04 | kg | |
| Energy inherent in ethanol | 3.44E+04 | MJ | |
| Gasoline that can replace the ethanol from corn | 7.91E+02 | kg | |
| | | | |
| Fuel consumption of a normal vehicle | 10 | l/100km | |
| Energy consumed per distance driven on gasoline | 301 | MJ/100km | |
| | 3.01 | MJ/km | |

## LCI for the expanded system boundaries

| Scenarios | | EE | HE | EE-HI | HE-HI | E-FFV | $H_2$-ICEV | E-FCV | $H_2$-FCV |
|---|---|---|---|---|---|---|---|---|---|
| Products | Units | | | | | | | | |
| | | | | | | | | | |
| Maize electricity | kWh | 3.14E+03 | 4.06E+03 | 3.14E+03 | 4.06E+03 | 0 | 0 | 0 | 0 |
| Coal added for maize electricity (heat) and (electricity) | MJ | 2.33E+04 | 2.47E+03 | 5.24E+02 | 0.00E+00 | 0 | 0 | 0 | 0 |
| | kWh | 7.00E+02 | 7.00E+02 | 7.00E+02 | 7.00E+02 | 0 | 0 | 0 | 0 |
| | | | | | | | | | |
| Maize Transport | km | 0 | 0 | 0 | 0 | 1.07E+04 | 1.66E+04 | 1.59E+04 | 3.22E+04 |
| Coal added for maize transport (heat) and (electricity) | MJ | 0 | 0 | 0 | 0 | 2.33E+04 | 2.47E+03 | 2.33E+04 | 2.47E+03 |
| | kWh | 0 | 0 | 0 | 0 | 7.00E+02 | 7.00E+02 | 7.00E+02 | 7.00E+02 |
| | | | | | | | | | |
| Coal based electricty added for system expansion | kWh | 9.22E+02 | 0 | 9.22E+02 | 0 | 4.06E+03 | 4.06E+03 | 4.06E+03 | 4.06E+03 |
| Coal added to generate coal electricity | kg | 4.37E+02 | 0 | 4.37E+02 | 0 | 1.93E+03 | 1.93E+03 | 1.93E+03 | 1.93E+03 |
| Amount of energy inherent in coal for electricity | MJ | 1.01E+04 | 0 | 1.01E+04 | 0 | 4.43E+04 | 4.43E+04 | 4.43E+04 | 4.43E+04 |
| Gasoline added for system expansion | km | 3.22E+04 | 3.22E+04 | 3.22E+04 | 3.22E+04 | 2.15E+04 | 1.55E+04 | 1.63E+04 | 0 |
| Gasoline added to achieve the mileage | kg | 2.23E+03 | 2.23E+03 | 2.23E+03 | 2.23E+03 | 1.49E+03 | 1.08E+03 | 1.13E+03 | 0 |
| | MJ | 9.69E+04 | 9.69E+04 | 9.69E+04 | 9.69E+04 | 6.46E+04 | 4.68E+04 | 4.91E+04 | 0 |

## Emissions associated with system expansion

| Item | Electrical Scenarios | E-FFV | $H_2$-ICEV | E-FCV | $H_2$- FCV |
|---|---|---|---|---|---|
| | kg | kg | kg | kg | kg |
| CO2 | 8.60E+03 | 5.74E+03 | 4.15E+03 | 4.36E+03 | 0.00E+00 |
| CH4 | 1.96E+00 | 1.31E+00 | 9.48E-01 | 9.95E-01 | 0.00E+00 |
| N2O | 3.63E-01 | 2.42E-01 | 1.75E-01 | 1.84E-01 | 0.00E+00 |
| GHGs | 8.75E+03 | 5.84E+03 | 4.23E+03 | 4.44E+03 | 0.00E+00 |
| VOC: Total | 5.82E+00 | 3.88E+00 | 2.81E+00 | 2.95E+00 | 0.00E+00 |
| CO: Total | 7.61E+01 | 5.08E+01 | 3.67E+01 | 3.86E+01 | 0.00E+00 |
| NOx: Total | 5.14E+00 | 3.43E+00 | 2.48E+00 | 2.61E+00 | 0.00E+00 |
| PM10: Total | 1.61E+00 | 1.07E+00 | 7.77E-01 | 8.16E-01 | 0.00E+00 |
| PM2.5: Total | 6.69E-01 | 4.46E-01 | 3.23E-01 | 3.39E-01 | 0.00E+00 |
| SOx: Total | 1.39E+00 | 9.27E-01 | 6.71E-01 | 7.05E-01 | 0.00E+00 |
| VOC: Urban | 3.65E+00 | 2.43E+00 | 1.76E+00 | 1.85E+00 | 0.00E+00 |
| CO: Urban | 4.72E+01 | 3.15E+01 | 2.28E+01 | 2.39E+01 | 0.00E+00 |
| NOx: Urban | 2.73E+00 | 1.82E+00 | 1.32E+00 | 1.38E+00 | 0.00E+00 |
| PM10: Urban | 5.48E-01 | 3.65E-01 | 2.65E-01 | 2.78E-01 | 0.00E+00 |
| PM2.5: Urban | 2.95E-01 | 1.97E-01 | 1.43E-01 | 1.50E-01 | 0.00E+00 |
| SOx: Urban | 6.82E-01 | 4.55E-01 | 3.29E-01 | 3.46E-01 | 0.00E+00 |

## Results of LCIA results from SimaPro

| Impact category | Unit | EE | EE-HI | E-FFV | E-FCV | HE | HE-HI | $H_2$-ICEV | $H_2$-FCV |
|---|---|---|---|---|---|---|---|---|---|
| global warming (GWP100) | kg CO2 eq | 1.05E-01 | 9.02E-02 | 1.01E-01 | 8.86E-02 | 8.54E-02 | 8.31E-02 | 7.34E-02 | 3.56E-02 |
| human toxicity | kg 1,4-DB eq | 6.67E-03 | 2.14E-03 | 1.05E-02 | 1.05E-02 | 1.60E-03 | 9.05E-04 | 6.23E-03 | 6.17E-03 |
| acidification | kg SO2 eq | 7.68E-04 | 1.41E-04 | 1.02E-03 | 1.02E-03 | 1.46E-04 | 4.92E-05 | 4.35E-04 | 4.35E-04 |
| fresh water aquatic ecotox. | kg 1,4-DB eq | 2.96E-04 | 1.84E-04 | 5.33E-04 | 5.26E-04 | 1.27E-04 | 1.10E-04 | 4.28E-04 | 3.99E-04 |
| eutrophication | kg PO4--- eq | 2.97E-04 | 2.92E-04 | 3.16E-04 | 3.14E-04 | 1.35E-04 | 1.35E-04 | 1.46E-04 | 1.40E-04 |

## $CO_2$ emissions contributions from various fossil products used for system expansion

| LCI input/output | EE | EE-HI | HE | HE-HI | E-FFV | E-FCV | H2-ICEV | H2-FCV |
|---|---|---|---|---|---|---|---|---|
| **Units** | **kg** | **kg** | **kg** | **kg** | **kg** | **kg** | **kg** | **kg** |
| Hard coal used for thermal requirements and coal based electricity | **1.34E+03** | **3.53E+02** | **4.38E+02** | **-** | **1.34E+03** | **1.34E+03** | **4.38E+02** | **4.38E+02** |
| | | | | | | | | |
| Electricity,ZA (Sys. Exp.) | **4.40E+02** | **4.40E+02** | **-** | **-** | **1.93E+03** | **1.93E+03** | **1.93E+03** | **1.93E+03** |
| Gasoline (Sys. Exp.) | **2.23E+03** | **2.23E+03** | **2.23E+03** | **2.23E+03** | **1.50E+03** | **1.13E+03** | **1.08E+03** | - |
| | | | | | | | | |
| $CO_{2\ gasoline}$ | **8.72E+03** | 8.72E+03 | 8.72E+03 | 8.72E+03 | 5.75E+03 | 4.37E+03 | 4.21E+03 | - |
| $CO_{2\ fuel\ production}$ | 1.70E+03 | 6.76E+01 | 2.53E+02 | 3.40E+00 | **1.77E+03** | 1.77E+03 | 2.55E+02 | 2.55E+02 |
| $CO_{2\ elec,\ ZA}$ | 1.11E+03 | 1.11E+03 | 4.78E+02 | 4.78E+02 | **3.29E+03** | 3.29E+03 | 3.28E+03 | 3.28E+03 |
| $CO_{2\ fossil\ (tot)}$ | **1.15E+04** | 9.90E+03 | 9.45E+03 | 9.20E+03 | 1.08E+04 | 9.44E+03 | 7.74E+03 | 3.53E+03 |
| $SO_{2\ equi.\ (fossil)}$ | 1.59E+01 | 5.74E+01 | 2.18E+01 | 6.07E+00 | **5.74E+01** | 5.66E+01 | 5.47E+01 | 5.15E+01 |
| $PO_{4\ equi.\ (fossil)}$ | 3.31E+01 | 3.23E+01 | 1.54E+01 | 2.00E+01 | **3.52E+01** | 3.50E+01 | 1.66E+01 | 1.60E+01 |

# Appendix A6: APR application in a coal to liquid Refinery

## Relevant equations

| | |
|---|---|
| $CO + H_2O \leftrightarrow CO_2 + H_2$ | Water-gas shift |
| $n[2H_2 + CO] \leftrightarrow (CH_2)n + nH_2O$ | General F-T equation |
| $16H_2 + 8CO \leftrightarrow C_8H_{16} + 8H_2O$ | F-T for gasoline production C8, where n=8 |

## Hydrogen from APR data

| | | |
|---|---|---|
| **Hydrogen produced from APR** | **173.86** | **kmol** |
| | **347.72** | **kg** |

## Gasoline production calculation

(Assumption that all the syngas gets converted to gasoline)

**Amount of Carbon dioxide needed to react with all APR hydrogen from a reference flow**

| | | |
|---|---|---|
| **Moles** | **5.74E+01** | **kmol** |
| **Mass** | **2.52E+03** | **kg** |
| Conversion | **33%** | |
| **Moles of CO produced** | **5.74E+01** | **kmol** |
| **Mass of CO produced** | **1.61E+03** | **kg** |
| **No of moles of H2 unreacted** | **1.16E+02** | **kmol** |
| **Molar ratio of H2/CO** | **2** | |
| Gasoline produced | **7.17** | **kmol** |
| | **8.18E+02** | **kg** |

## Calculations for the mileage driven with gasoline produced from APR H2

| | | |
|---|---|---|
| Fuel consumption of a normal vehicle | **10** | **l/100km** |
| | **0.1** | **l/km** |
| Density of gasoline | **0.692** | **kg/l** |
| Volume of ethanol produced | **1.18E+03** | **l** |
| Milleage driven on a gasoline vehicle | **1.18E+04** | **km** |

## Carbon dioxide avoided per day

| | | |
|---|---|---|
| Carbon dioxide from emissions | 5.74E+01 | kmol |
| | 2.52E+03 | kg |
| | 2.52 | tons/ton |

| Components | Input flows | | Output flows | |
|---|---|---|---|---|
| | kg | kmol | kg | kmol |
| Hydrogen | 3.48E+02 | 1.74E+02 | - | - |
| Carbon dioxide | 7.65E+03 | 1.74E+02 | 1.16E+02 | |
| Carbon monoxide | - | - | | |
| Gasoline | - | - | | |
| Water | - | - | | |

| | | Hydrogen | Carbon dioxide | Carbon monoxide | Gasoline | Water |
|---|---|---|---|---|---|---|
| | | | | | | |
| **W-G shift input** | kg | **3.48E+02** | **7.65E+03** | **-** | **-** | **-** |
| | kmol | **1.74E+02** | **1.74E+02** | **-** | **-** | **-** |
| | | | | | | |
| **W-G shift outlet** | kg | **2.33E+02** | **5.13E+03** | **1.61E+03** | **-** | **1.61E+03** |
| | kmol | **1.16E+02** | **1.16E+02** | **5.74E+01** | **-** | **5.74E+01** |
| | | | | | | |
| **F-T reactor outlet** | kg | **-** | **-** | **-** | **8.18E+02** | **1.03E+03** |
| | kmol | **-** | **-** | **-** | **7.17** | **5.74E+01** |
| | l | **-** | **-** | **-** | **1.18E+03** | **1.03E+03** |

## System Expansion for the 5 transport

| Item | Fuel production g/mile | Vehicle Operation g/mile |
|---|---|---|
| CO2 | **7.19E+01** | **3.56E+02** |

GREET 1.7

**1 ton** 1000 kg
**1 mile** 1.6 km

| Tranport options | E-FFV | C-L ICEV | E-FCV | H2-ICEV | H2-FCV |
|---|---|---|---|---|---|
| | | | | | |
| km driven | **1.07E+04** | **1.18E+04** | **1.66E+04** | **1.59E+04** | **3.22E+04** |

| | | E-FFV | H2-ICEV | E-FCV | H2-FCV | CTL-H2 |
|---|---|---|---|---|---|---|
| Maize Transport | **km** | **1.07E+04** | **1.59E+04** | **1.66E+04** | **3.22E+04** | **1.18E+04** |
| | **MJ** | 2.33E+04 | 2.47E+03 | 2.33E+04 | 2.47E+03 | 2.47E+03 |
| | **kWh** | 7.00E+02 | 7.00E+02 | 7.00E+02 | 7.00E+02 | 7.00E+02 |
| Expansion | **km added** | 2.15E+04 | 1.63E+04 | 1.55E+04 | 0.00E+00 | 3.22E+04 |
| Conversion of km added into $CO_2$ emissions | **t** | 5.74 | 4.36 | 4.15 | 0.00 | 8.60 |
| CO2 emissions from fuel prod. | **t** | 2.20 | 0.74 | 2.19 | 0.74 | 0.74 |
| Mileage on CTL | **km** | **1.18E+04** | **1.18E+04** | **1.18E+04** | **1.18E+04** | **1.18E+04** |
| tailpipe (ex CTL) | **t** | 2.70 | 2.70 | 2.70 | 2.70 | 2.70 |
| production (ex CTL) | **t** | 2.52 | 2.52 | 2.52 | 2.52 | 0.00 |
| Tot. $CO_2$ | **t** | **13.15** | **10.32** | **11.56** | **5.96** | **12.04** |
| **Total mileage** | | **4.40E+04** | **4.40E+04** | **4.40E+04** | **4.40E+04** | **4.40E+04** |